

Four-center Integral of a Dipolar Two-electron Potential Between s -type GTO's

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We reduce two-electron 4-center products of Cartesian Gaussian Type Orbitals with Boys' contraction to 2-center products of the form $\psi_\alpha(\mathbf{r}_i - \mathbf{A}) \psi_\beta(\mathbf{r}_j - \mathbf{B})$, and compute the 6-dimensional integral over $d^3r_i d^3r_j$ over these with the effective potential $V_{ij} = (\mathbf{r}_i - \mathbf{r}_j) \cdot \mathbf{r}_j / |\mathbf{r}_i - \mathbf{r}_j|^3$ in terms of Shavitt's confluent hypergeometric functions.

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I. FORMAT OF THE INTEGRAL

In relativistic quantum chemistry, the effective electron-electron interaction contains so-called gauge correction terms [1–3] which appear in the computation as energy integrals of the form

$$J(\alpha, \mathbf{A}, \beta, \mathbf{B}, \gamma, \mathbf{C}, \delta, \mathbf{D}) = \int d^3r_i d^3r_j \psi_\alpha(\mathbf{r}_i - \mathbf{A}) \psi_\beta(\mathbf{r}_i - \mathbf{B}) \frac{(\mathbf{r}_i - \mathbf{r}_j) \cdot (2\mathbf{r}_i - \mathbf{r}_j)}{|\mathbf{r}_i - \mathbf{r}_j|^3} \psi_\gamma(\mathbf{r}_j - \mathbf{C}) \psi_\delta(\mathbf{r}_j - \mathbf{D}) \quad (1)$$

for orbitals ψ centered at places \mathbf{A} , \mathbf{B} , \mathbf{C} and \mathbf{D} . The Gauss Transformation Method has been shown to calculate the integral if the orbitals ψ are expanded in a basis of Gaussian Type Orbitals (GTO's) [4]; this manuscript basically demonstrates how dealing with the quadratic forms in the exponentials directly also manages to reduce them to the omnipresent Confluent Hypergeometric Functions of the electron repulsion integrals (ERI's).

II. REDUCTION TO 2-CENTER INTEGRALS

By the usual treatment of GTO's [5] we contract the Gaussians related to electron i and electron j by defining intermediate centers \mathbf{P} and \mathbf{Q} :

$$\mathbf{P} \equiv \frac{\alpha\mathbf{A} + \beta\mathbf{B}}{\alpha + \beta}, \quad (2)$$

$$\mathbf{Q} \equiv \frac{\gamma\mathbf{C} + \delta\mathbf{D}}{\gamma + \delta}, \quad (3)$$

$$e^{-\alpha(\mathbf{r}-\mathbf{A})^2} e^{-\beta(\mathbf{r}-\mathbf{B})^2} = \exp\left[-\frac{\alpha\beta}{\alpha+\beta}(\mathbf{A}-\mathbf{B})^2\right] e^{-(\alpha+\beta)(\mathbf{r}-\mathbf{P})^2}, \quad (4)$$

$$e^{-\gamma(\mathbf{r}-\mathbf{C})^2} e^{-\delta(\mathbf{r}-\mathbf{D})^2} = \exp\left[-\frac{\gamma\delta}{\gamma+\delta}(\mathbf{C}-\mathbf{D})^2\right] e^{-(\gamma+\delta)(\mathbf{r}-\mathbf{Q})^2}. \quad (5)$$

Prefactors of the form $(x_i - A_x)^{n_x\alpha} (y_i - A_y)^{n_y\alpha} (z_i - A_z)^{n_z\alpha} (x_i - B_x)^{n_x\beta} (y_i - B_y\beta)^{n_y} (z_i - B_z)^{n_z\beta}$ introduced by Cartesian GTO's of higher angular momentum quantum numbers n_x , n_y and n_z are also re-centered at \mathbf{P} and \mathbf{Q} by binomial expansion [6]. Hermite Gaussians or Spherical Gaussians may be re-centered by transformation to and from an intermediate Cartesian basis for the same goal [7].

After that step the integrals are 2-center integrals:

$$\bar{J} \equiv \exp\left[-\frac{\alpha\beta}{\alpha+\beta}(\mathbf{A}-\mathbf{B})^2 - \frac{\gamma\delta}{\gamma+\delta}(\mathbf{C}-\mathbf{D})^2\right] I(\kappa, \mathbf{P}, \lambda, \mathbf{Q}), \quad (6)$$

where

$$I(\kappa, \mathbf{P}, \lambda, \mathbf{Q}) \equiv \int d^3r_i d^3r_j \psi_\kappa(\mathbf{r}_i - \mathbf{P}) \frac{(\mathbf{r}_i - \mathbf{r}_j) \cdot (2\mathbf{r}_i - \mathbf{r}_j)}{|\mathbf{r}_i - \mathbf{r}_j|^3} \psi_\lambda(\mathbf{r}_j - \mathbf{Q}). \quad (7)$$

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III. REDUCTION TO A TRIPLE INTEGRAL

The substitution $\mathbf{R} = \mathbf{r}_i - \mathbf{r}_j$ in the integrand of the previous equation yields

$$I = \int d^3 R d^3 r_j \psi_\kappa(\mathbf{R} + \mathbf{r}_j - \mathbf{P}) \frac{\mathbf{R} \cdot (2\mathbf{R} + \mathbf{r}_j)}{R^3} \psi_\lambda(\mathbf{r}_j - \mathbf{Q}). \quad (8)$$

A. Isotropic Term

The first term of $I = K + \bar{I}$ in the previous equation is the well known 2-electron Coulomb repulsion [8]:

$$\begin{aligned} K &\equiv \int d^3 R d^3 r_j \psi_\kappa(\mathbf{R} + \mathbf{r}_j - \mathbf{P}) \frac{\mathbf{R} \cdot 2\mathbf{R}}{R^3} \psi_\lambda(\mathbf{r}_j - \mathbf{Q}) = 2 \int d^3 R d^3 r_j \psi_\kappa(\mathbf{R} + \mathbf{r}_j - \mathbf{P}) \frac{1}{R} \psi_\lambda(\mathbf{r}_j - \mathbf{Q}) \\ &= 2e^{-\kappa P^2 - \lambda Q^2} \int dr_x dr_y dr_z dR_x dR_y dR_z \\ &\times e^{-\kappa[R_x^2 + R_y^2 + R_z^2 + r_x^2 + r_y^2 + r_z^2 + 2R_x r_x + 2R_y r_y + 2R_z r_z - 2R_x P_x - 2R_y P_y - 2R_z P_z - 2r_x P_x - 2r_y P_y - 2r_z P_z]} \\ &\times \frac{1}{(R_x^2 + R_y^2 + R_z^2)^{1/2}} e^{-\lambda[r_x^2 + r_y^2 + r_z^2 - 2r_x Q_x - 2r_y Q_y - 2r_z Q_z]} \\ &= 2e^{-\kappa P^2 - \lambda Q^2} \left[\int dr_x dR_x \int dr_y dR_y \int dr_z dR_z e^{-\kappa[R_x^2 + r_x^2 + 2R_x r_x - 2R_x P_x - 2r_x P_x]} \right. \\ &\quad \times e^{-\kappa[R_y^2 + r_y^2 + 2R_y r_y - 2R_y P_y - 2r_y P_y]} \\ &\quad \times e^{-\kappa[R_z^2 + r_z^2 + 2R_z r_z - 2R_z P_z - 2r_z P_z]} \\ &\quad \times \frac{1}{(R_x^2 + R_y^2 + R_z^2)^{1/2}} e^{-\lambda[r_x^2 - 2r_x Q_x]} e^{-\lambda[r_y^2 - 2r_y Q_y]} e^{-\lambda[r_z^2 - 2r_z Q_z]} \left. \right] \\ &= 2e^{-\kappa P^2 - \lambda Q^2} \left[\int dr_x dR_x e^{-\kappa[R_x^2 + r_x^2 + 2R_x r_x - 2R_x P_x - 2r_x P_x]} \frac{1}{(R_x^2 + R_y^2 + R_z^2)^{1/2}} e^{-\lambda[r_x^2 - 2r_x Q_x]} \right. \\ &\quad \times \int dr_y dR_y e^{-\kappa[R_y^2 + r_y^2 + 2R_y r_y - 2R_y P_y - 2r_y P_y]} e^{-\lambda[r_y^2 - 2r_y Q_y]} \\ &\quad \times \left. \int dr_z dR_z e^{-\kappa[R_z^2 + r_z^2 + 2R_z r_z - 2R_z P_z - 2r_z P_z]} e^{-\lambda[r_z^2 - 2r_z Q_z]} \right]. \quad (9) \end{aligned}$$

The integral over r_z is handled as usual by completion of the quadratic form of r_z in the exponential

$$\begin{aligned} \int dr_z e^{-\kappa[R_z^2 + r_z^2 + 2R_z r_z - 2R_z P_z - 2r_z P_z]} e^{-\lambda[r_z^2 - 2r_z Q_z]} &= e^{-\kappa[R_z^2 - 2R_z P_z]} \int dr_z e^{-\kappa[r_z^2 + 2R_z r_z - 2r_z P_z] - \lambda[r_z^2 - 2r_z Q_z]} \\ &= e^{-\kappa[R_z^2 - 2R_z P_z]} \int dr_z e^{-(\kappa + \lambda)r_z^2 - 2\kappa R_z r_z + 2\kappa r_z P_z + 2\lambda r_z Q_z} = e^{-\kappa[R_z^2 - 2R_z P_z]} \int dr_z e^{-(\kappa + \lambda)r_z^2 - 2(\kappa R_z - \kappa P_z - \lambda Q_z)r_z} \\ &= e^{-\kappa[R_z^2 - 2R_z P_z]} \int dr_z e^{-(\kappa + \lambda)[r_z^2 + 2\frac{\kappa R_z - \kappa P_z - \lambda Q_z}{\kappa + \lambda} r_z]} \\ &= e^{-\kappa[R_z^2 - 2R_z P_z]} \int dr_z e^{-(\kappa + \lambda)[r_z^2 + 2\frac{\kappa R_z - \kappa P_z - \lambda Q_z}{\kappa + \lambda} r_z + (\frac{\kappa R_z - \kappa P_z - \lambda Q_z}{\kappa + \lambda})^2 - (\frac{\kappa R_z - \kappa P_z - \lambda Q_z}{\kappa + \lambda})^2]} \\ &= e^{-\kappa[R_z^2 - 2R_z P_z]} e^{-(\kappa + \lambda)[-(\frac{\kappa R_z - \kappa P_z - \lambda Q_z}{\kappa + \lambda})^2]} \int dr_z e^{-(\kappa + \lambda)[r_z^2 + 2\frac{\kappa R_z - \kappa P_z - \lambda Q_z}{\kappa + \lambda} r_z + (\frac{\kappa R_z - \kappa P_z - \lambda Q_z}{\kappa + \lambda})^2]} \\ &= e^{-\kappa[R_z^2 - 2R_z P_z]} e^{(\kappa + \lambda)(\frac{\kappa R_z - \kappa P_z - \lambda Q_z}{\kappa + \lambda})^2} \int dr_z e^{-(\kappa + \lambda)r_z^2} \\ &= e^{-\kappa[R_z^2 - 2R_z P_z]} e^{\frac{(\kappa R_z - \kappa P_z - \lambda Q_z)^2}{\kappa + \lambda}} \sqrt{\frac{\pi}{\kappa + \lambda}}. \quad (10) \end{aligned}$$

The same treatment integrates along the r_x and the r_y directions:

$$\int dr_x e^{-\kappa[R_x^2 + r_x^2 + 2R_x r_x - 2R_x P_x - 2r_x P_x]} e^{-\lambda[r_x^2 - 2r_x Q_x]} = e^{-\kappa[R_x^2 - 2R_x P_x]} e^{\frac{(\kappa R_x - \kappa P_x - \lambda Q_x)^2}{\kappa + \lambda}} \sqrt{\frac{\pi}{\kappa + \lambda}}. \quad (11)$$

$$\int dr_y e^{-\kappa[R_y^2+r_y^2+2R_y r_y-2R_y P_y-2r_y P_y]} e^{-\lambda[r_y^2-2r_y Q_y]} = e^{-\kappa[R_y^2-2R_y P_y]} e^{\frac{(\kappa R_y-\kappa P_y-\lambda Q_y)^2}{\kappa+\lambda}} \sqrt{\frac{\pi}{\kappa+\lambda}}. \quad (12)$$

Insertion of the previous three equations into (9) yields

$$\begin{aligned} K = 2e^{-\kappa P^2-\lambda Q^2} \left(\frac{\pi}{\kappa+\lambda}\right)^{3/2} \int dR_x dR_y dR_z e^{-\kappa[R_x^2-2R_x P_x]} e^{\frac{(\kappa R_x-\kappa P_x-\lambda Q_x)^2}{\kappa+\lambda}} \\ \times e^{-\kappa[R_y^2-2R_y P_y]} e^{\frac{(\kappa R_y-\kappa P_y-\lambda Q_y)^2}{\kappa+\lambda}} \\ \times e^{-\kappa[R_z^2-2R_z P_z]} e^{\frac{(\kappa R_z-\kappa P_z-\lambda Q_z)^2}{\kappa+\lambda}} \frac{1}{(R_x^2+R_y^2+R_z^2)^{1/2}}. \end{aligned} \quad (13)$$

The principal axis transformation in the Gaussian exponentials with the main variable R_x is

$$e^{-\kappa[R_x^2-2R_x P_x]} e^{\frac{(\kappa R_x-\kappa P_x-\lambda Q_x)^2}{\kappa+\lambda}} = \exp[\kappa P_x^2 + \lambda Q_x^2] \exp\left[-\frac{\kappa\lambda}{\kappa+\lambda}(R_x - P_x + Q_x)^2\right]. \quad (14)$$

Substitution of this form for R_x , R_y and R_z into (13) produces

$$\begin{aligned} K = 2e^{-\kappa P^2-\lambda Q^2} \left(\frac{\pi}{\kappa+\lambda}\right)^{3/2} \int dR_x dR_y dR_z \exp[\kappa P_x^2 + \lambda Q_x^2] \exp\left[-\frac{\kappa\lambda}{\kappa+\lambda}(R_x - P_x + Q_x)^2\right] \\ \times \exp[\kappa P_y^2 + \lambda Q_y^2] \exp\left[-\frac{\kappa\lambda}{\kappa+\lambda}(R_y - P_y + Q_y)^2\right] \\ \times \exp[\kappa P_z^2 + \lambda Q_z^2] \exp\left[-\frac{\kappa\lambda}{\kappa+\lambda}(R_z - P_z + Q_z)^2\right] \frac{1}{(R_x^2+R_y^2+R_z^2)^{1/2}} \\ = 2\left(\frac{\pi}{\kappa+\lambda}\right)^{3/2} \int dR_x dR_y dR_z \exp\left[-\frac{\kappa\lambda}{\kappa+\lambda}(R_x - P_x + Q_x)^2\right] \\ \times \exp\left[-\frac{\kappa\lambda}{\kappa+\lambda}(R_y - P_y + Q_y)^2\right] \\ \times \exp\left[-\frac{\kappa\lambda}{\kappa+\lambda}(R_z - P_z + Q_z)^2\right] \frac{1}{(R_x^2+R_y^2+R_z^2)^{1/2}}. \end{aligned} \quad (15)$$

Definition of a new vector \mathbf{E} and of a reduced scaling parameter ϵ

$$\mathbf{E} \equiv \mathbf{P} - \mathbf{Q}, \quad \epsilon \equiv \frac{\kappa\lambda}{\kappa+\lambda}, \quad (16)$$

expresses (15) as an integral over the entire space of d^3R :

$$K = 2\left(\frac{\pi}{\kappa+\lambda}\right)^{3/2} \int dR_x dR_y dR_z \exp[-\epsilon(\mathbf{R} - \mathbf{E})^2] \frac{1}{(R_x^2+R_y^2+R_z^2)^{1/2}}. \quad (17)$$

We rotate the coordinate system such that the vector \mathbf{E} points along the polar coordinate and switch to a spherical coordinate system with radial coordinate X , polar coordinate θ and azimuth ϕ . A factor $X^2 \sin \theta$ from the Jacobian

in spherical coordinates is inserted,

$$\begin{aligned}
K(\epsilon, \mathbf{E}) &= 2\left(\frac{\pi}{\kappa + \lambda}\right)^{3/2} e^{-\epsilon E^2} \int X^2 \sin \theta dX d\theta d\phi \exp[-\epsilon\{X^2 - 2EX \cos \theta\}] \frac{1}{X} \\
&= 2\left(\frac{\pi}{\kappa + \lambda}\right)^{3/2} e^{-\epsilon E^2} \int X \sin \theta dX d\theta d\phi \exp[-\epsilon\{X^2 - 2EX \cos \theta\}] \\
&= 2\left(\frac{\pi}{\kappa + \lambda}\right)^{3/2} 2\pi e^{-\epsilon E^2} \int X \sin \theta dX d\theta \exp[-\epsilon\{X^2 - 2EX \cos \theta\}] \\
&= 2\left(\frac{\pi}{\kappa + \lambda}\right)^{3/2} 2\pi e^{-\epsilon E^2} \int X dX \int_{-1}^1 dz \exp[-\epsilon\{X^2 - 2EXz\}] \\
&= 2\left(\frac{\pi}{\kappa + \lambda}\right)^{3/2} 2\pi e^{-\epsilon E^2} \int_0^\infty X dX e^{-\epsilon X^2} \int_{-1}^1 dz \exp[2\epsilon EXz] \\
&= 2\left(\frac{\pi}{\kappa + \lambda}\right)^{3/2} 2\pi e^{-\epsilon E^2} \int_0^\infty X dX e^{-\epsilon X^2} \frac{1}{2\epsilon EX} (e^{2\epsilon EX} - e^{-2\epsilon EX}) \\
&= 2\left(\frac{\pi}{\kappa + \lambda}\right)^{3/2} \frac{\pi}{\epsilon E} e^{-\epsilon E^2} \int_0^\infty dX e^{-\epsilon X^2} (e^{2\epsilon EX} - e^{-2\epsilon EX}) \\
&= 2\left(\frac{\pi}{\kappa + \lambda}\right)^{3/2} \frac{\pi}{2\epsilon^2 E^2} e^{-\epsilon E^2} \int_0^\infty dt e^{-t^2/(4\epsilon E^2)} (e^t - e^{-t}) = 2\left(\frac{\pi}{\kappa + \lambda}\right)^{3/2} \frac{2\pi}{\epsilon} F_0(\epsilon E^2). \quad (18)
\end{aligned}$$

The function F_0 is made more explicit in Appendix B.

B. Dipolar Term

The entire focus of this manuscript is on the second term of I in (8),

$$\bar{I}(\kappa, \mathbf{P}, \lambda, \mathbf{Q}) \equiv \int d^3R d^3r_j \psi_\kappa(\mathbf{R} + \mathbf{r}_j - \mathbf{P}) \frac{\mathbf{R} \cdot \mathbf{r}_j}{R^3} \psi_\lambda(\mathbf{r}_j - \mathbf{Q}). \quad (19)$$

For s -type orbitals along the Cartesian coordinates $\mathbf{r}_j = (r_x, r_y, r_z)$ the dot product $\mathbf{R} \cdot \mathbf{r}_j$ is expanded which

decomposes \bar{I} into a sum of three contributions:

$$\begin{aligned}
\bar{I}(\kappa, \mathbf{P}, \lambda, \mathbf{Q}) &= e^{-\kappa P^2 - \lambda Q^2} \int dr_x dr_y dr_z dR_x dR_y dR_z \\
&\quad \times e^{-\kappa[R_x^2 + R_y^2 + R_z^2 + r_x^2 + r_y^2 + r_z^2 + 2R_x r_x + 2R_y r_y + 2R_z r_z - 2R_x P_x - 2R_y P_y - 2R_z P_z - 2r_x P_x - 2r_y P_y - 2r_z P_z]} \\
&\quad \times \frac{R_x r_x + R_y r_y + R_z r_z}{(R_x^2 + R_y^2 + R_z^2)^{3/2}} e^{-\lambda[r_x^2 + r_y^2 + r_z^2 - 2r_x Q_x - 2r_y Q_y - 2r_z Q_z]} \\
&= e^{-\kappa P^2 - \lambda Q^2} \left[\int dr_x dr_y dr_z dR_x dR_y dR_z e^{-\kappa[R_x^2 + R_y^2 + R_z^2 + r_x^2 + r_y^2 + r_z^2 + 2R_x r_x + 2R_y r_y + 2R_z r_z - 2R_x P_x - 2R_y P_y - 2R_z P_z - 2r_x P_x - 2r_y P_y - 2r_z P_z]} \right. \\
&\quad \times \frac{R_x r_x}{(R_x^2 + R_y^2 + R_z^2)^{3/2}} e^{-\lambda[r_x^2 + r_y^2 + r_z^2 - 2r_x Q_x - 2r_y Q_y - 2r_z Q_z]} \\
&\quad + \int dr_x dr_y dr_z dR_x dR_y dR_z e^{-\kappa[R_x^2 + R_y^2 + R_z^2 + r_x^2 + r_y^2 + r_z^2 + 2R_x r_x + 2R_y r_y + 2R_z r_z - 2R_x P_x - 2R_y P_y - 2R_z P_z - 2r_x P_x - 2r_y P_y - 2r_z P_z]} \\
&\quad \times \frac{R_y r_y}{(R_x^2 + R_y^2 + R_z^2)^{3/2}} e^{-\lambda[r_x^2 + r_y^2 + r_z^2 - 2r_x Q_x - 2r_y Q_y - 2r_z Q_z]} \\
&\quad + \left. \int dr_x dr_y dr_z dR_x dR_y dR_z e^{-\kappa[R_x^2 + R_y^2 + R_z^2 + r_x^2 + r_y^2 + r_z^2 + 2R_x r_x + 2R_y r_y + 2R_z r_z - 2R_x P_x - 2R_y P_y - 2R_z P_z - 2r_x P_x - 2r_y P_y - 2r_z P_z]} \right. \\
&\quad \times \left. \frac{R_z r_z}{(R_x^2 + R_y^2 + R_z^2)^{3/2}} e^{-\lambda[r_x^2 + r_y^2 + r_z^2 - 2r_x Q_x - 2r_y Q_y - 2r_z Q_z]} \right] \\
&= e^{-\kappa P^2 - \lambda Q^2} \left[\int dr_x dR_x \int dr_y dR_y \int dr_z dR_z e^{-\kappa[R_x^2 + r_x^2 + 2R_x r_x - 2R_x P_x - 2r_x P_x]} \right. \\
&\quad \times e^{-\kappa[R_y^2 + r_y^2 + 2R_y r_y - 2R_y P_y - 2r_y P_y]} \\
&\quad \times e^{-\kappa[R_z^2 + r_z^2 + 2R_z r_z - 2R_z P_z - 2r_z P_z]} \\
&\quad \times \frac{R_x r_x}{(R_x^2 + R_y^2 + R_z^2)^{3/2}} e^{-\lambda[r_x^2 - 2r_x Q_x]} e^{-\lambda[r_y^2 - 2r_y Q_y]} e^{-\lambda[r_z^2 - 2r_z Q_z]} \\
&\quad \left. + (x \rightarrow y) + (x \rightarrow z) \right] \\
&= e^{-\kappa P^2 - \lambda Q^2} \left[\int dr_x dR_x e^{-\kappa[R_x^2 + r_x^2 + 2R_x r_x - 2R_x P_x - 2r_x P_x]} \frac{R_x r_x}{(R_x^2 + R_y^2 + R_z^2)^{3/2}} e^{-\lambda[r_x^2 - 2r_x Q_x]} \right. \\
&\quad \times \int dr_y dR_y e^{-\kappa[R_y^2 + r_y^2 + 2R_y r_y - 2R_y P_y - 2r_y P_y]} e^{-\lambda[r_y^2 - 2r_y Q_y]} \\
&\quad \times \int dr_z dR_z e^{-\kappa[R_z^2 + r_z^2 + 2R_z r_z - 2R_z P_z - 2r_z P_z]} e^{-\lambda[r_z^2 - 2r_z Q_z]} \\
&\quad \left. + (x \rightarrow y) + (x \rightarrow z) \right]. \quad (20)
\end{aligned}$$

The integrals over r_z and r_y are taken from (10) and (12). An additional factor r_x intrudes the integrand along the

r_x -direction in (20):

$$\begin{aligned}
& \int dr_x r_x e^{-\kappa[R_x^2+r_x^2+2R_x r_x-2R_x P_x-2r_x P_x]} e^{-\lambda[r_x^2-2r_x Q_x]} \\
&= e^{-\kappa[R_x^2-2R_x P_x]} e^{-(\kappa+\lambda)\left[-\left(\frac{\kappa R_x-\kappa P_x-\lambda Q_x}{\kappa+\lambda}\right)^2\right]} \int dr_x r_x e^{-(\kappa+\lambda)\left[r_x^2+2\frac{\kappa R_x-\kappa P_x-\lambda Q_x}{\kappa+\lambda}r_x+\left(\frac{\kappa R_x-\kappa P_x-\lambda Q_x}{\kappa+\lambda}\right)^2\right]} \\
&= e^{-\kappa[R_x^2-2R_x P_x]} e^{(\kappa+\lambda)\left[\left(\frac{\kappa R_x-\kappa P_x-\lambda Q_x}{\kappa+\lambda}\right)^2\right]} \int dr_x r_x e^{-(\kappa+\lambda)\left[r_x+\frac{\kappa R_x-\kappa P_x-\lambda Q_x}{\kappa+\lambda}\right]^2} \\
&= e^{-\kappa[R_x^2-2R_x P_x]} e^{(\kappa+\lambda)\left[\left(\frac{\kappa R_x-\kappa P_x-\lambda Q_x}{\kappa+\lambda}\right)^2\right]} \int dt \left(t-\frac{\kappa R_x-\kappa P_x-\lambda Q_x}{\kappa+\lambda}\right) e^{-(\kappa+\lambda)t^2} \\
&= -\frac{\kappa R_x-\kappa P_x-\lambda Q_x}{\kappa+\lambda} e^{-\kappa[R_x^2-2R_x P_x]} e^{\frac{(\kappa R_x-\kappa P_x-\lambda Q_x)^2}{\kappa+\lambda}} \int dt e^{-(\kappa+\lambda)t^2} \\
&= -\frac{\kappa R_x-\kappa P_x-\lambda Q_x}{\kappa+\lambda} e^{-\kappa[R_x^2-2R_x P_x]} e^{\frac{(\kappa R_x-\kappa P_x-\lambda Q_x)^2}{\kappa+\lambda}} \sqrt{\frac{\pi}{\kappa+\lambda}}. \quad (21)
\end{aligned}$$

Insertion of this equation, of (12) and of (10) into (20) has reduced the 6-fold to a 3-fold integral:

$$\begin{aligned}
\bar{I} = e^{-\kappa P^2-\lambda Q^2} & \left[-\left(\frac{\pi}{\kappa+\lambda}\right)^{3/2} \int dR_x dR_y dR_z \frac{\kappa R_x-\kappa P_x-\lambda Q_x}{\kappa+\lambda} e^{-\kappa[R_x^2-2R_x P_x]} e^{\frac{(\kappa R_x-\kappa P_x-\lambda Q_x)^2}{\kappa+\lambda}} \right. \\
& \times e^{-\kappa[R_y^2-2R_y P_y]} e^{\frac{(\kappa R_y-\kappa P_y-\lambda Q_y)^2}{\kappa+\lambda}} \\
& \times e^{-\kappa[R_z^2-2R_z P_z]} e^{\frac{(\kappa R_z-\kappa P_z-\lambda Q_z)^2}{\kappa+\lambda}} \frac{R_x}{(R_x^2+R_y^2+R_z^2)^{3/2}} \\
& \left. + (x \rightarrow y) + (x \rightarrow z) \right]. \quad (22)
\end{aligned}$$

IV. REDUCTION OF THE 1-PARTICLE POTENTIAL

A. Quadratic Form in the Exponential

Substitution of the form (14) for R_x , R_y and R_z into (22) produces

$$\begin{aligned}
\bar{I} = e^{-\kappa P^2-\lambda Q^2} & \left[-\left(\frac{\pi}{\kappa+\lambda}\right)^{3/2} \int dR_x dR_y dR_z \frac{\kappa R_x-\kappa P_x-\lambda Q_x}{\kappa+\lambda} \exp[\kappa P_x^2+\lambda Q_x^2] \exp\left[-\frac{\kappa\lambda}{\kappa+\lambda}(R_x-P_x+Q_x)^2\right] \right. \\
& \times \exp[\kappa P_y^2+\lambda Q_y^2] \exp\left[-\frac{\kappa\lambda}{\kappa+\lambda}(R_y-P_y+Q_y)^2\right] \\
& \times \exp[\kappa P_z^2+\lambda Q_z^2] \exp\left[-\frac{\kappa\lambda}{\kappa+\lambda}(R_z-P_z+Q_z)^2\right] \frac{R_x}{(R_x^2+R_y^2+R_z^2)^{3/2}} \\
& \left. + (R_x \rightarrow R_y) + (R_x \rightarrow R_z) \right] \\
& = -\left(\frac{\pi}{\kappa+\lambda}\right)^{3/2} \int dR_x dR_y dR_z \frac{\kappa R_x-\kappa P_x-\lambda Q_x}{\kappa+\lambda} \exp\left[-\frac{\kappa\lambda}{\kappa+\lambda}(R_x-P_x+Q_x)^2\right] \\
& \times \exp\left[-\frac{\kappa\lambda}{\kappa+\lambda}(R_y-P_y+Q_y)^2\right] \\
& \times \exp\left[-\frac{\kappa\lambda}{\kappa+\lambda}(R_z-P_z+Q_z)^2\right] \frac{R_x}{(R_x^2+R_y^2+R_z^2)^{3/2}} \\
& \left. + (R_x \rightarrow R_y) + (R_x \rightarrow R_z) \right]. \quad (23)
\end{aligned}$$

Along with (16),

$$\begin{aligned} \bar{I} &= -\left(\frac{\pi}{\kappa + \lambda}\right)^{3/2} \int dR_x dR_y dR_z \frac{\kappa R_x - \kappa P_x - \lambda Q_x}{\kappa + \lambda} \exp\left[-\frac{\kappa\lambda}{\kappa + \lambda}(\mathbf{R} - \mathbf{E})^2\right] \frac{R_x}{(R_x^2 + R_y^2 + R_z^2)^{3/2}} \\ &\quad + (R_x \rightarrow R_y) + (R_x \rightarrow R_z) \\ &= -\left(\frac{\pi}{\kappa + \lambda}\right)^{3/2} \int dR_x dR_y dR_z \frac{\kappa \mathbf{R} \cdot \mathbf{R} - (\kappa \mathbf{P} + \lambda \mathbf{Q}) \cdot \mathbf{R}}{\kappa + \lambda} \exp[-\epsilon(\mathbf{R} - \mathbf{E})^2] \frac{1}{(R_x^2 + R_y^2 + R_z^2)^{3/2}}. \end{aligned} \quad (24)$$

The exponent in this integrand involves the cosine of the angle between the vectors \mathbf{R} and \mathbf{E} ,

$$\exp[-\epsilon(\mathbf{R} - \mathbf{E})^2] = \exp[-\epsilon\{R^2 + E^2 - 2ER(\sin\theta \sin\theta_E \cos(\phi - \phi_E) + \cos\theta \cos\theta_E)\}] \quad (25)$$

where polar and azimuthal angles are defined in the usual manner:

$$\mathbf{R} = R(\sin\theta \cos\phi, \sin\theta \sin\phi, \cos\theta); \quad (26)$$

$$\mathbf{E} = E(\sin\theta_E \cos\phi_E, \sin\theta_E \sin\phi_E, \cos\theta_E). \quad (27)$$

As the only noticeable idea in this calculation, the inverse coordinate transformation (A5) rotates the R -coordinate system such that the polar axis of the new coordinate system points towards \mathbf{E} , so the cosine in the dot product $\mathbf{R} \cdot \mathbf{E}$ is just the cosine of the polar coordinate of \mathbf{X} in the new coordinate system observed in (A2):

$$\mathbf{R} = \mathbf{\Omega}^{-1} \mathbf{X}; \quad (28)$$

$$\mathbf{R} \cdot \mathbf{E} = \mathbf{\Omega}^{-1} \mathbf{X} \cdot \mathbf{E} = \mathbf{X} \cdot \mathbf{\Omega} \mathbf{E}. \quad (29)$$

$$\mathbf{\Omega}^{-1} = \begin{pmatrix} (1 - \cos\theta_E) \sin^2\phi_E + \cos\theta_E & -(1 - \cos\theta_E) \sin\phi_E \cos\phi_E & \sin\theta_E \cos\phi_E \\ -(1 - \cos\theta_E) \cos\phi_E \sin\phi_E & (1 - \cos\theta_E) \cos^2\phi_E + \cos\theta_E & \sin\theta_E \sin\phi_E \\ -\sin\theta_E \cos\phi_E & -\sin\theta_E \sin\phi_E & \cos\theta_E \end{pmatrix}. \quad (30)$$

The rotation preserves lengths, $R = |\mathbf{R}| = X = |\mathbf{X}|$.

$$\bar{I} = -\left(\frac{\pi}{\kappa + \lambda}\right)^{3/2} \int dX_x dX_y dX_z \frac{\kappa \mathbf{X} \cdot \mathbf{X} - (\kappa \mathbf{P} + \lambda \mathbf{Q}) \cdot \mathbf{\Omega}^{-1} \mathbf{X}}{\kappa + \lambda} \exp[-\epsilon(\mathbf{\Omega}^{-1} \mathbf{X} - \mathbf{E})^2] \frac{1}{(X_x^2 + X_y^2 + X_z^2)^{3/2}} \quad (31)$$

$$= -\left(\frac{\pi}{\kappa + \lambda}\right)^{3/2} \int dX_x dX_y dX_z \left(\frac{\kappa}{\kappa + \lambda} X^2 - \mathbf{E}' \cdot \mathbf{\Omega}^{-1} \mathbf{X}\right) \exp[-\epsilon(\mathbf{\Omega}^{-1} \mathbf{X} - \mathbf{E})^2] \frac{1}{(X_x^2 + X_y^2 + X_z^2)^{3/2}} \quad (32)$$

$$= -\left(\frac{\pi}{\kappa + \lambda}\right)^{3/2} \left[\frac{\kappa}{\kappa + \lambda} \bar{I}_1 - \bar{I}_2\right], \quad (33)$$

where we have defined the vector \mathbf{E}' via

$$\mathbf{E}' \equiv \frac{\kappa \mathbf{P} + \lambda \mathbf{Q}}{\kappa + \lambda}. \quad (34)$$

B. Isotropic Part

The term \bar{I}_1 in (33) involves a factor $X^2 \sin \theta$ from the Jacobian in spherical coordinates, a factor $\mathbf{X} \cdot \mathbf{X} = X^2$ from the dot product, and the dipolar X^3 in the denominator:

$$\begin{aligned}
\bar{I}_1(\epsilon, \mathbf{E}) &= \int dX_x dX_y dX_z X^2 \exp[-\epsilon(\mathbf{X} - \mathbf{E})^2] \frac{1}{(X_x^2 + X_y^2 + X_z^2)^{3/2}} \\
&= e^{-\epsilon E^2} \int X^2 \sin \theta dX d\theta d\phi X^2 \exp[-\epsilon\{X^2 - 2EX \cos \theta\}] \frac{1}{(X_x^2 + X_y^2 + X_z^2)^{3/2}} \\
&= e^{-\epsilon E^2} \int X \sin \theta dX d\theta d\phi \exp[-\epsilon\{X^2 - 2EX \cos \theta\}] \\
&= 2\pi e^{-\epsilon E^2} \int X \sin \theta dX d\theta \exp[-\epsilon\{X^2 - 2EX \cos \theta\}] \\
&= 2\pi e^{-\epsilon E^2} \int X dX \int_{-1}^1 dz \exp[-\epsilon\{X^2 - 2EXz\}] \\
&= 2\pi e^{-\epsilon E^2} \int_0^\infty X dX e^{-\epsilon X^2} \int_{-1}^1 dz \exp[2\epsilon EXz] \\
&= 2\pi e^{-\epsilon E^2} \int_0^\infty X dX e^{-\epsilon X^2} \frac{1}{2\epsilon EX} (e^{2\epsilon EX} - e^{-2\epsilon EX}) \\
&= \frac{\pi}{\epsilon E} e^{-\epsilon E^2} \int_0^\infty dX e^{-\epsilon X^2} (e^{2\epsilon EX} - e^{-2\epsilon EX}) \\
&= \frac{\pi}{2\epsilon^2 E^2} e^{-\epsilon E^2} \int_0^\infty dt e^{-t^2/(4\epsilon E^2)} (e^t - e^{-t}) = \frac{2\pi}{\epsilon} F_0(\epsilon E^2). \quad (35)
\end{aligned}$$

The function F_0 is made more explicit in Appendix B. The gradient with respect to \mathbf{E} is an application of (D2):

$$\nabla_{\mathbf{E}} \bar{I}_1 = -4\pi F_1(\epsilon E^2) \mathbf{E}. \quad (36)$$

This indicates that working out the integrals for 4-center orbitals of Cartesian Gaussians beyond the (0,0,0)-triple of ‘‘orbital’’ quantum numbers are tractable through repeated differentiation with respect to the locations of the four centers [9, 10].

C. Dipolar Part

In the other integral of (33),

$$\bar{I}_2 = \int d^3 X \mathbf{E}' \cdot \boldsymbol{\Omega}^{-1} \mathbf{X} \exp[-\epsilon(\boldsymbol{\Omega}^{-1} \mathbf{X} - \mathbf{E})^2] \frac{1}{X^3},$$

we compute three components defined by moving the $\boldsymbol{\Omega}$ operator to the vector \mathbf{E}' :

$$\mathbf{E}' \cdot \boldsymbol{\Omega}^{-1} \mathbf{X} = \boldsymbol{\Omega} \mathbf{E}' \cdot \mathbf{X} = H_x X_x + H_y X_y + H_z X_z \quad (37)$$

where we have defined the vector $\mathbf{H} \equiv \boldsymbol{\Omega} \mathbf{E}'$.

$$\bar{I}_2 = H_x \bar{I}_{2x} + H_y \bar{I}_{2y} + H_z \bar{I}_{2z}. \quad (38)$$

Its z -component is obtained with (A5):

$$H_z = \frac{1}{E} \mathbf{E} \cdot \mathbf{E}'. \quad (39)$$

The integrals \bar{I}_{2x} and \bar{I}_{2y} vanish while integrating over the azimuth ϕ :

$$\begin{aligned}
\bar{I}_{2x} &= \int dX_x dX_y dX_z X_x \exp\left[-\frac{\kappa\lambda}{\kappa+\lambda}(\boldsymbol{\Omega}^{-1} \mathbf{X} - \mathbf{E})^2\right] \frac{1}{(X_x^2 + X_y^2 + X_z^2)^{3/2}} \\
&= e^{-\epsilon E^2} \int dX \sin \theta d\theta d\phi \cos \phi \sin \theta \exp[-\epsilon\{X^2 - 2EX \cos \theta\}] = 0. \quad (40)
\end{aligned}$$

$$\begin{aligned}\bar{I}_{2y} &= \int dX_x dX_y dX_z X_y \exp\left[-\frac{\kappa\lambda}{\kappa+\lambda}(\boldsymbol{\Omega}^{-1}\mathbf{X} - \mathbf{E})^2\right] \frac{1}{(X_x^2 + X_y^2 + X_z^2)^{3/2}} \\ &= e^{-\epsilon E^2} \int dX \sin\theta d\theta d\phi \sin\phi \sin\theta \exp[-\epsilon\{X^2 - 2EX\cos\theta\}] = 0.\end{aligned}\quad (41)$$

So the only finite contribution to (38) is from the component coupled to H_z :

$$\begin{aligned}\bar{I}_{2z}(\epsilon, \mathbf{E}) &= \int dX_x dX_y dX_z X_z \exp\left[-\frac{\kappa\lambda}{\kappa+\lambda}(\boldsymbol{\Omega}^{-1}\mathbf{X} - \mathbf{E})^2\right] \frac{1}{(X_x^2 + X_y^2 + X_z^2)^{3/2}} \\ &= e^{-\epsilon E^2} \int dX \sin\theta d\theta d\phi \cos\theta \exp[-\epsilon\{X^2 - 2EX\cos\theta\}] \\ &= 2\pi e^{-\epsilon E^2} \int dX \sin\theta d\theta \cos\theta \exp[-\epsilon\{X^2 - 2EX\cos\theta\}] \\ &= 2\pi e^{-\epsilon E^2} \int_0^\infty dX \int_{-1}^1 dt \exp[-\epsilon\{X^2 - 2EXt\}] \\ &= 2\pi e^{-\epsilon E^2} \int_0^\infty dX e^{-\epsilon X^2} \int_{-1}^1 dt \exp[2\epsilon EXt] \\ &= 2\pi e^{-\epsilon E^2} \int_0^\infty dX e^{-\epsilon X^2} \frac{1}{(2\epsilon EX)^2} [e^{2\epsilon EX}(2\epsilon EX - 1) + e^{-2\epsilon EX}(2\epsilon EX + 1)] \\ &= 2\pi e^{-\epsilon E^2} \frac{1}{2\epsilon E} \int_0^\infty dt e^{-t^2/(4\epsilon E^2)} \frac{1}{t^2} [e^t(t-1) + e^{-t}(t+1)] = 4\pi E F_1(\epsilon E^2).\end{aligned}\quad (42)$$

The auxiliary special function F_1 is computed via the error function in Appendix C. The gradient with respect to \mathbf{E} is an application of (D2) and of the product rule of differentiation:

$$\nabla_{\mathbf{E}} \bar{I}_{2z} = \frac{4\pi}{E} [F_1(\epsilon E^2) - 2\epsilon E^2 F_2(\epsilon E^2)] \mathbf{E}.\quad (43)$$

V. SUMMARY

In numerical practise the steps of obtaining J are:

1. Define the intermediate centers \mathbf{P} and \mathbf{Q} with their effective scaling factors $\kappa + \beta$ and $\lambda + \delta$ via (2) and (3);
2. Calculate the exponential pre-factor in (6);
3. Implement Shavitt's functions F_0 and F_1 for positive real-valued arguments;
4. Calculate the contribution K with (18);
5. Calculate the contribution \bar{I} from (33):
 - (a) Calculate the two vectors \mathbf{E} , \mathbf{E}' and parameter ϵ in (16) and (34);
 - (b) Calculate $\bar{I}_2 = H_z \bar{I}_{2z}$ as the product of (39) and (42).
 - (c) Calculate \bar{I}_1 in (35).
6. Calculate (7)

$$I = K + \bar{I} = \frac{2\pi}{\epsilon} \left(\frac{\pi}{\kappa + \lambda}\right)^{3/2} \left[\frac{\kappa + 2\lambda}{\kappa + \lambda} F_0(\epsilon E^2) + 2\epsilon \mathbf{E} \cdot \mathbf{E}' F_1(\epsilon E^2) \right].\quad (44)$$

Appendix A: Coordinate rotation

The orthogonal unimodular 3×3 matrix which rotates points by an angle θ_E around the right-handed axis with Cartesian coordinates $(\omega_1, \omega_2, \omega_3)$, normalized to unit length $\omega_1^2 + \omega_2^2 + \omega_3^2 = 1$, is [11][12, (2.21)]

$$\mathbf{\Omega} = \begin{pmatrix} (1 - \cos \theta_E)\omega_1^2 + \cos \theta_E & (1 - \cos \theta_E)\omega_1\omega_2 - \sin \theta_E\omega_3 & (1 - \cos \theta_E)\omega_1\omega_3 + \sin \theta_E\omega_2 \\ (1 - \cos \theta_E)\omega_1\omega_2 + \sin \theta_E\omega_3 & (1 - \cos \theta_E)\omega_2^2 + \cos \theta_E & (1 - \cos \theta_E)\omega_2\omega_3 - \sin \theta_E\omega_1 \\ (1 - \cos \theta_E)\omega_1\omega_3 - \sin \theta_E\omega_2 & (1 - \cos \theta_E)\omega_2\omega_3 + \sin \theta_E\omega_1 & (1 - \cos \theta_E)\omega_3^2 + \cos \theta_E \end{pmatrix}. \quad (\text{A1})$$

We wish to find the axis that rotates the Cartesian vector (27) to the image $E(0, 0, 1)$, such that

$$\mathbf{\Omega} \cdot \begin{pmatrix} \cos \phi_E \sin \theta_E \\ \sin \phi_E \sin \theta_E \\ \cos \theta_E \end{pmatrix} = \begin{pmatrix} 0 \\ 0 \\ 1 \end{pmatrix}. \quad (\text{A2})$$

The rotation axis is the cross product between the point in space and its image:

$$\begin{pmatrix} \cos \phi_E \sin \theta_E \\ \sin \phi_E \sin \theta_E \\ \cos \theta_E \end{pmatrix} \times \begin{pmatrix} 0 \\ 0 \\ 1 \end{pmatrix} = \begin{pmatrix} \sin \phi_E \sin \theta_E \\ -\cos \phi_E \sin \theta_E \\ 0 \end{pmatrix}. \quad (\text{A3})$$

Normalized to unit length it constructs the axis vector ω with Cartesian components

$$\begin{pmatrix} \omega_1 \\ \omega_2 \\ \omega_3 \end{pmatrix} = \begin{pmatrix} \sin \phi_E \\ -\cos \phi_E \\ 0 \end{pmatrix}. \quad (\text{A4})$$

Insertion of these three components into (A1) yields the rotation matrix applicable to (A2):

$$\mathbf{\Omega} = \begin{pmatrix} (1 - \cos \theta_E) \sin^2 \phi_E + \cos \theta_E & -(1 - \cos \theta_E) \sin \phi_E \cos \phi_E & -\sin \theta_E \cos \phi_E \\ -(1 - \cos \theta_E) \cos \phi_E \sin \phi_E & (1 - \cos \theta_E) \cos^2 \phi_E + \cos \theta_E & -\sin \theta_E \sin \phi_E \\ \sin \theta_E \cos \phi_E & \sin \theta_E \sin \phi_E & \cos \theta_E \end{pmatrix}. \quad (\text{A5})$$

The inverse rotation is represented by the inverse matrix (which equals the transpose matrix) and established through the substitution $\theta_E \rightarrow -\theta_E$.

Appendix B: Auxiliary Integral F_0

The radial integral (18) resp. (35) is solved by Taylor Expansion of the $\sinh t$, followed by the substitution $t^2 = s$ and integration over s with [13, 3.351.3]

$$\int_0^\infty e^{-s/k} s^n ds = n! k^{n+1}. \quad (\text{B1})$$

$$\begin{aligned} F_0(k) &\equiv \frac{1}{4k} e^{-k} \int_0^\infty dt e^{-t^2/(4k)} (e^t - e^{-t}) = \frac{1}{4k} e^{-k} \int_0^\infty dt e^{-t^2/(4k)} 2 \sum_{l=1,3,5,\dots} \frac{t^l}{l!} \\ &= \frac{1}{4k} e^{-k} \int_0^\infty ds e^{-s/(4k)} \sum_{l \geq 0} \frac{s^l}{(2l+1)!} \\ &= \frac{1}{4k} e^{-k} \sum_{l \geq 0} \frac{l!}{(2l+1)!} (4k)^{l+1} \\ &= e^{-k} \sum_{l \geq 0} \frac{[\Gamma(l+1)]^2 (4k)^l}{\Gamma(2l+2) l!}. \quad (\text{B2}) \end{aligned}$$

Application of the duplication formula for the Γ -function [14, 6.1.18] and rewriting the Γ -functions as Pochhammer symbols converts the series to a Confluent Hypergeometric Function [15, 16]:

$$F_0(k) = e^{-k} {}_1F_1(1; 3/2; k) = {}_1F_1(1/2; 3/2; -k) = \frac{1}{2}k^{-1/2}\gamma(1/2, k) = \frac{1}{2}k^{-1/2}\sqrt{\pi}\operatorname{erf}(\sqrt{k}). \quad (\text{B3})$$

For small arguments the Taylor expansion is [14, 7.1.5]

$$F_0(k) \xrightarrow{k \rightarrow 0} 1 - \frac{1}{3}k + \frac{1}{10}k^2 - \frac{1}{42}k^3 + \frac{1}{108}k^4 + \dots \quad (\text{B4})$$

Appendix C: Auxiliary Integral F_1

The auxiliary function introduced in (42) for real-valued argument $k \geq 0$ turns out to be closely related to the error function [17]. Very similar to the calculation in Appendix B, the exponentials in the integral that depend linearly on t are expanded in Taylor series [13, 1.212], summation and integration are interchanged, and integration via (B1) yields a Confluent Hypergeometric Series:

$$\begin{aligned} F_1(k) &= \frac{1}{4k}e^{-k} \int_0^\infty dt e^{-t^2/(4k)} \frac{1}{t^2} [e^{-t}(1+t) + e^t(t-1)] \\ &= \frac{1}{4k}e^{-k} \int_0^\infty dt e^{-t^2/(4k)} 2 \sum_{l \geq 0} t^{2l+1} \frac{2l+2}{(2l+3)!} \\ &= \frac{1}{4k}e^{-k} \int_0^\infty ds e^{-s/(4k)} \sum_{l \geq 0} s^l \frac{2l+2}{(2l+3)!} \\ &= \frac{1}{4k}e^{-k} \sum_{l \geq 0} (4k)^{l+1} \frac{(2l+2)l!}{(2l+3)!} \\ &= 2e^{-k} \sum_{l \geq 0} \frac{(l+1)!! (4k)^l}{(2l+3)! l!} = \frac{1}{3}e^{-k} {}_1F_1(1; 5/2; k). \quad (\text{C1}) \end{aligned}$$

Kummer's transformation [13, 9.212] and a succession of well-known formulas for the Incomplete Gamma-function [14, 13.1.27, 13.6.10, 6.5.22] rephrase F_1 in terms of the error function:

$$F_1(k) = \frac{1}{3} {}_1F_1(3/2; 5/2; -k) = \frac{1}{2}k^{-3/2} \left[\frac{\sqrt{\pi}}{2} \operatorname{erf}(\sqrt{k}) - \sqrt{k}e^{-k} \right]. \quad (\text{C2})$$

For small arguments [14, 7.1.5]

$$F_1(k) \xrightarrow{k \rightarrow 0} \frac{1}{3} - \frac{1}{5}k + \frac{1}{14}k^2 - \frac{1}{54}k^3 + \frac{1}{264}k^4 + \dots \quad (\text{C3})$$

Appendix D: Shavitt's F -integral

F_0 and F_1 are special cases of Shavitt's F_ν -functions [18–24]

$$F_\nu(t) \equiv \int_0^1 u^{2\nu} e^{-tu^2} du = \frac{1}{2\nu+1} {}_1F_1(\nu + \frac{1}{2}; \nu + \frac{3}{2}; -t) = \frac{1}{2\nu+1} e^{-t} {}_1F_1(1; \nu + \frac{3}{2}; t). \quad (\text{D1})$$

Its first derivative is

$$\frac{d}{dt} F_\nu(t) = -F_{\nu+1}(t). \quad (\text{D2})$$

The recurrence of the Confluent Hypergeometric Function [14, 13.4.7]

$$b(1-b+z) {}_1F_1(a; b; z) + b(b-1) {}_1F_1(a-1; b-1; z) - az {}_1F_1(a+1; b+1; z) = 0 \quad (\text{D3})$$

TABLE I. Coefficients $\beta_{\nu,l}$ in (D8) in row ν and column l . $\beta_{\nu,l} = 0$ if $l > \nu$, above the diagonal.

	0	1	2	3	4	5	6	7
0	-1							
1	1	1						
2	-3	-3	-1					
3	15	15	6	1				
4	-105	-105	-45	-10	-1			
5	945	945	420	105	15	1		
6	-10395	-10395	-4725	-1260	-210	-21	-1	
7	135135	135135	62370	17325	3150	378	28	1

establishes through insertion of $a = \nu + 3/2$, $b = \nu + 5/2$ the equivalent

$$zF_{\nu+2}(z) - (z + \nu + 3/2)F_{\nu+1}(z) + (\nu + 1/2)F_{\nu}(z) = 0. \quad (\text{D4})$$

The Laplace transform is

$$\hat{F}_{\nu}(s) \equiv \int_0^{\infty} e^{-st} F_{\nu}(t) dt = \int_0^1 \frac{1}{s+u^2} du u^{2\nu}, \quad (\text{D5})$$

with recurrence

$$\hat{F}_{\nu+1}(s) = \frac{1}{2\nu+1} - s\hat{F}_{\nu}(s), \quad (\text{D6})$$

starting at

$$\hat{F}_0(s) = \int_0^1 \frac{1}{s+u^2} du = \frac{1}{\sqrt{s}} \arctan \frac{1}{\sqrt{s}}. \quad (\text{D7})$$

The only singularity of $\hat{F}_{\nu}(s)$ is at $s = 0$.

By performing the analysis of (B2) or (C1) backwards we find for general integer ν

$$\begin{aligned} F_{\nu}(k) &= \frac{1}{2\nu+1} e^{-k} \sum_{l \geq 0} \frac{(1)_l k^l}{(\nu+3/2)_l l!} \\ &= \frac{e^{-k}}{4k} \frac{2}{2\nu+1} \int_0^{\infty} dt e^{-t^2/(4k)} t_0 F_1(-; \nu+3/2; t^2/4) \\ &= \frac{e^{-k}}{4k} (2\nu-1)!! 2 \sum_{l \geq 0} \int_0^{\infty} dt e^{-t^2/(4k)} \frac{1}{t^{2\nu}} t^{2\nu+2l+1} \frac{(2l+2)(2l+4) \cdots (2l+2\nu)}{(2\nu+1+2l)!} \\ &= (2\nu-1)!! \frac{e^{-k}}{4k} \int_0^{\infty} dt e^{-t^2/(4k)} \frac{1}{t^{2\nu}} [e^{-t}(\beta_{\nu,0} + \beta_{\nu,1}t + \beta_{\nu,2}t^2 + \beta_{\nu,3}t^3 + \cdots) - (t \rightarrow -t)]. \quad (\text{D8}) \end{aligned}$$

The absolute values of the matrix elements $\beta_{\nu,l}$ are Sequence A001497 in the Online Encyclopedia of Integer Sequences [25], illustrated in Table I. The row $\nu = 0$ in the table represents (B2), the row $\nu = 1$ represents (C1). The closed form

$$\beta_{\nu,l} = \begin{cases} (-1)^{\nu+1} 2^{l-\nu} \frac{\nu!}{l!} \binom{2\nu-l}{\nu}^{-1}, & 0 \leq l \leq \nu; \\ 0, & \text{else.} \end{cases} \quad (\text{D9})$$

is readily available [25]. The matrix inverse of β is also a lower triangular array with elements essentially obtained by transposition of β itself:

$$(\beta^{-1})_{\nu,l} = \begin{cases} (-1)^{\nu+1} |\beta_{1+l,1-\nu+2l}|, & \lfloor \nu/2 \rfloor \leq l \leq \nu; \\ 0, & \text{else.} \end{cases} \quad (\text{D10})$$

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