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Resolutions of the Coulomb Operator

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The "Resolution of the Identity Operator"

$$\hat{I} \equiv |\chi_n\rangle\langle\chi_n| \tag{1}$$

is a mathematical device that can be used to decouple the bra and ket in an overlap matrix element

$$\langle f|g\rangle = \langle f|\chi_n\rangle\langle\chi_n|g\rangle \tag{2}$$

through the introduction of an infinite complete expansion basis $\{\chi_n\}$. In practical implementations, where the basis set is finite and incomplete, (2) yields systematic approximations to difficult overlap integrals and is widely used in quantum physics and chemistry. We will present an analogous "Resolution of the Coulomb Operator"

$$r_{12}^{-1} \equiv |\phi_n\rangle\langle\phi_n| \tag{3}$$

which allows one to expand Coulomb matrix elements

$$\langle f|r_{12}^{-1}|g\rangle = \langle f|\phi_n\rangle\langle\phi_n|g\rangle \tag{4}$$

and we will discuss the potential utility of (4) in the efficient treatment of the matrix elements that arise in quantum chemistry and elsewhere.