Evaluation of exchange integrals by Fourier transform
of the 1/r operator and its numerical quadrature

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This contribution deals with the use of the old idea to replace the $1/r_{12}$ operator by the Fourier transform. If numerical quadrature is applied instead of derivation of formulas for analytical calculation, we obtain

$$\int f_1(\mathbf{r_1})\frac{1}{r_{12}}f_2(\mathbf{r_2})\mathrm{d}\mathbf{r_1}\mathrm{d}\mathbf{r_2} = \frac{1}{2\pi^2}\sum_{p}^{radial}\sum_{j}^{angular}\omega_p\omega_j(f_1(\mathbf{r_1})\exp(-\mathbf{k_{p,j}}\mathbf{r_1}))(f_2(\mathbf{r_2})\exp(\mathbf{k_{p,j}}\mathbf{r_2})),$$

where ω_p and ω_j are weights of roots of the numerical quadrature and expressions in parentheses are overlap integrals for functions f and plane-wave functions. The stimulus for this study arose from a need to evaluate efficiently exchange integrals of the type $(g_1(1)k_1(1)|g_2(2)k_2(2))$, where g's and k's, respectively, are gaussians and plane-wave functions. Evaluation of these integrals is still a bottleneck in *ab initio* calculations on electron scattering by polyatomic molecules. The objective of this contribution is to show that this way of evaluation of exchange integrals may be also beneficial for the mainstream quantum chemistry. For securing a needed accuracy of integrals the expansion of 1/r in plane-wave functions must be very large, but the formulas for overlap (gk) integrals and their analytical derivatives are simple and their evaluation is very fast. It will be shown that in spite of their large number considerable computer time saving may be achieved. This opens a way to treatments of electron scattering by larger molecules than it was possible so far. Possibly time saving may also be obtained in this way for the exchange energy in a pure Gaussian basis.