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A series expansion of the Coulomb operator for optimization scheme of the multi-reference density functional theory KOICHI KUSAKABE, ISAO MARUYAMA, Graduate School of Engineering Science, Osaka University — A quadratic form of the Coulomb operator for the many-electron system is derived.[1] This form of the electron-electron interaction is a sum of quadratic form pairs, which can be redefined in a self-consistent calculation of the multi-reference density functional theory. By virtue of this finding, the extended Kohn-Sham scheme[2] is shown to possess an optimization scheme of the effective electron model, which converges on the exact Coulomb system. For a defined accuracy of computation with given numerical technique, we can provide an algorithm to have an optimized electron model. The present procedure provides also an exact derivation of effective negative interactions in charge fluctuation channels. Relevance to the high-temperature superconductors is discussed. [1] K. Kusakabe, to appear in J. Phys.: Condens. Matter. [2] K. Kusakabe, J. Phys. Soc. Jpn. 70, 2038 (2001).

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