

SPLITTING OF THE COULOMB KERNEL
IN THE MULTILEVEL FAST
SUMMATION METHOD

*N. Gloskovskaya, V. Ilyin*¹

Bogolyubov Institute for Theoretical Physics,
Nat. Acad. Sci. of Ukraine
(*Kyiv 03143, Ukraine*),

¹Department of Computer Science
and Applied Mathematics,
The Weizmann Institute of Science
(*Rehovot 76100, Israel*)

S u m m a r y

A family of Coulomb kernels smoothed with even order polynomials is studied in the framework of the multilevel approach to the calculation of the interaction energy between particles. It is shown that the Ewald decomposition of the Coulomb potential is close to the polynomial softening with the order $8 \div 12$. It follows from the multilevel estimation of the Madelung constant, that, for a small cut-off radius, the better accuracy can be attained by using polynomials of smaller order. Therefore, these polynomials are computationally inexpensive to evaluate in the fast summation methods.