Efficient solution of Poisson's equation with free boundary conditions

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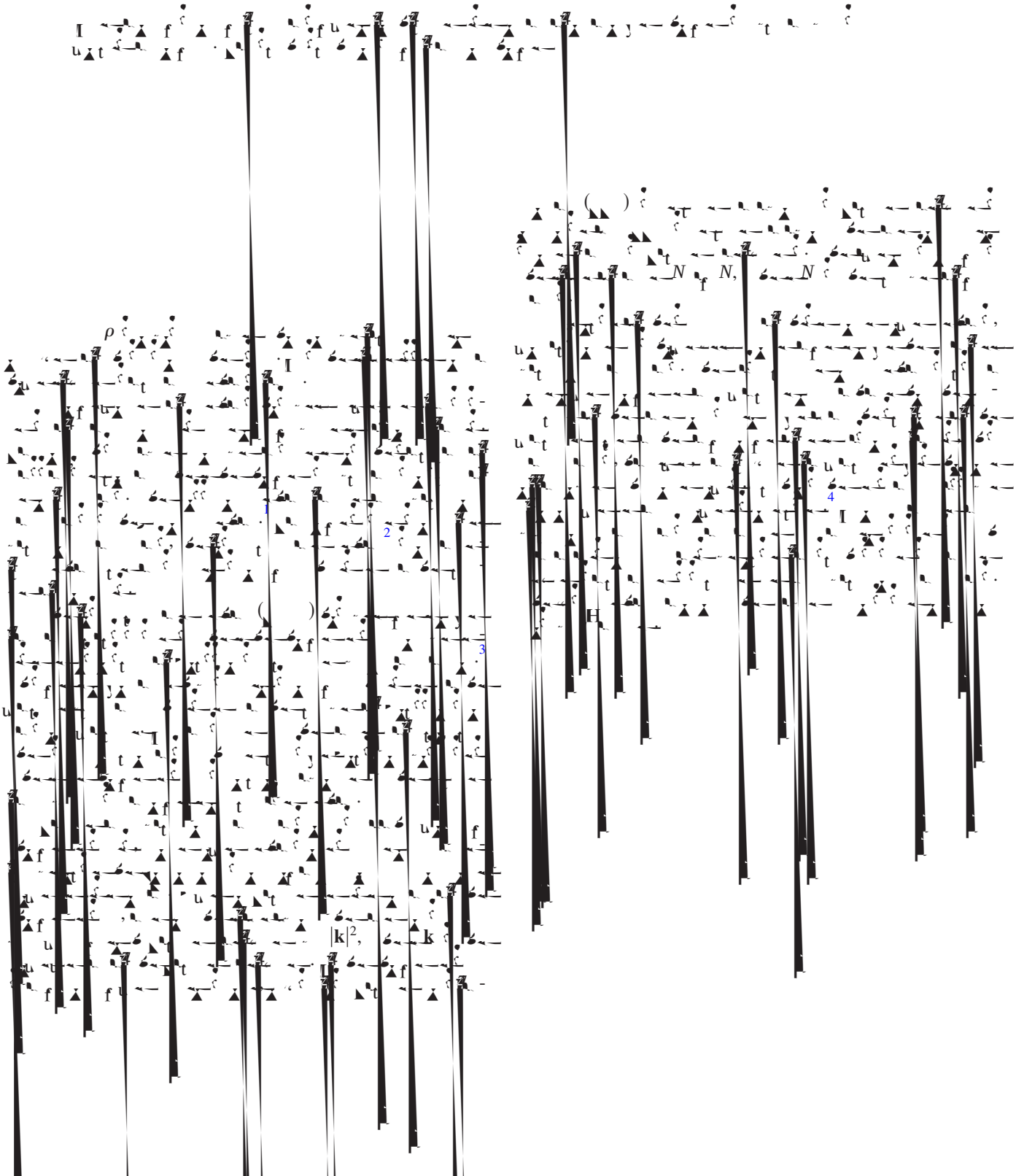
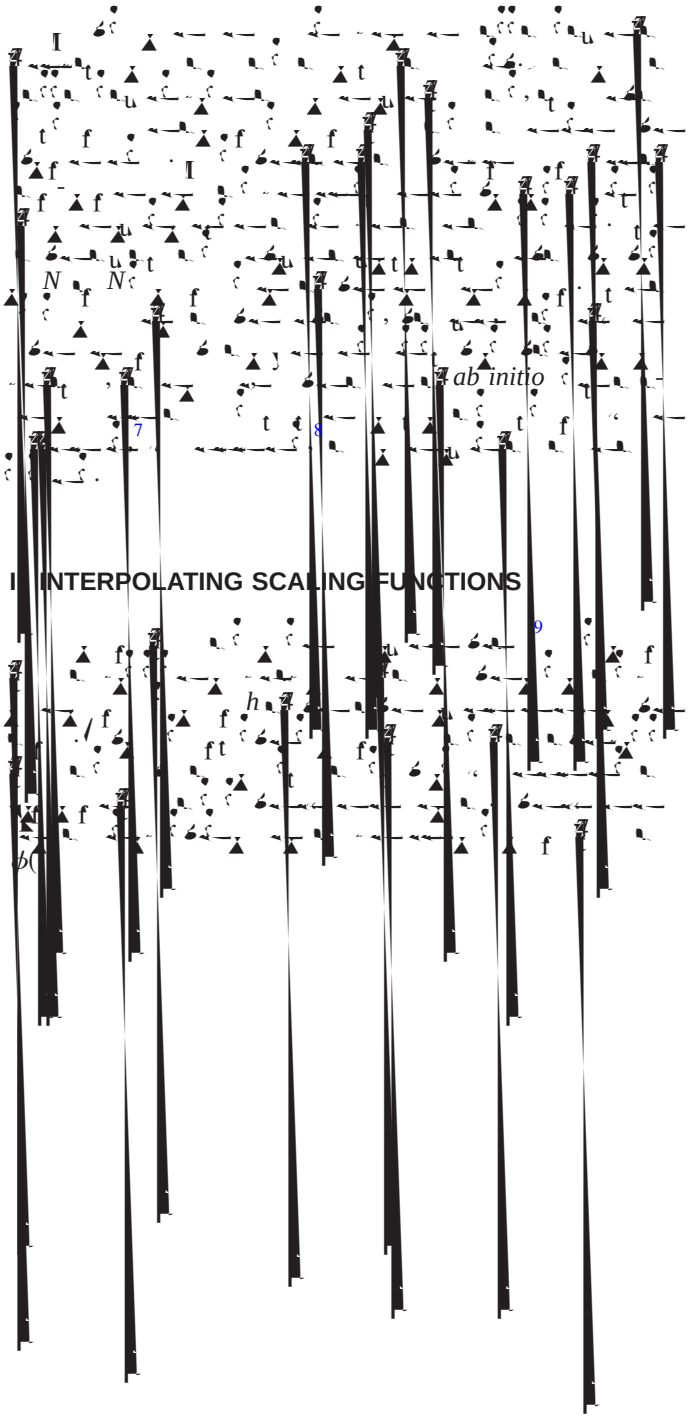




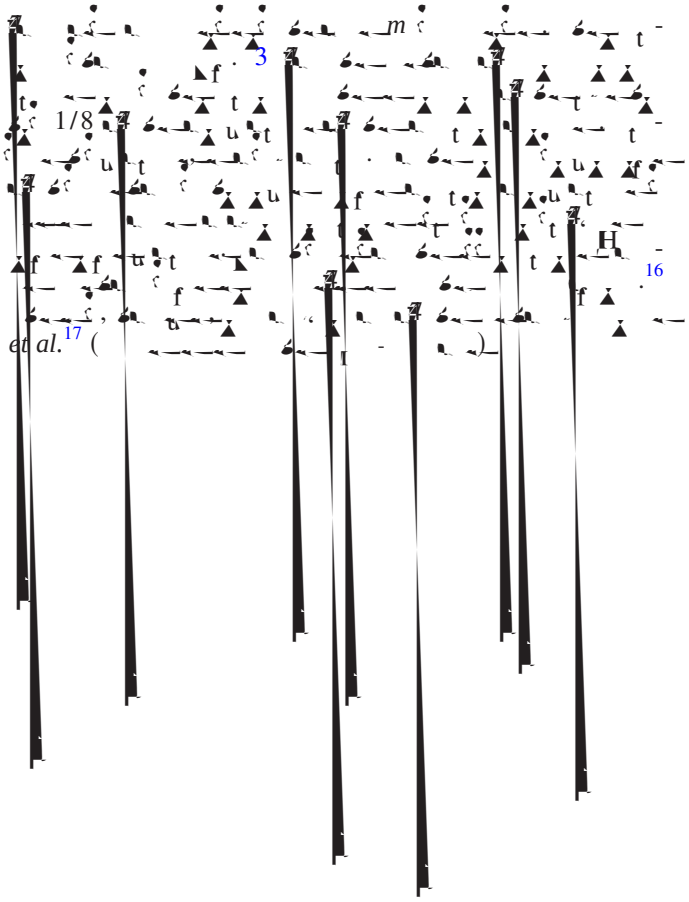
ab initio

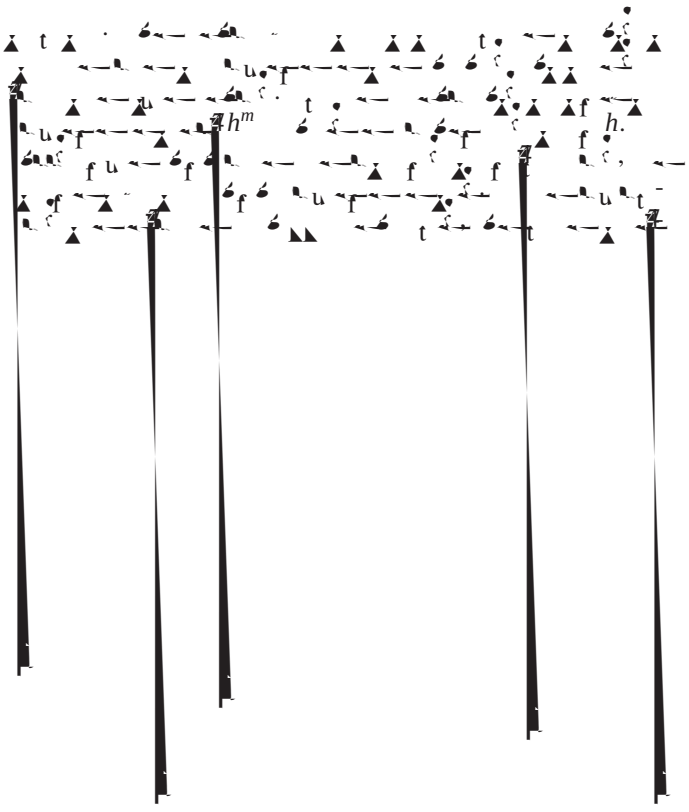
II. INTERPOLATING SCALING FUNCTIONS

$\mathbf{r}_{j_1,j_2,j_3} = (x_{j_1}, y_{j_2}, z_{j_3})$ V_{j_1,j_2,j_3}

$= V(\mathbf{r}_{j_1 j_2,j_3}),$

V_{jj}





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APPENDIX: PROOF OF EQ. (6)

(6). $\phi(x)$ m, ρ_{i_1,i_2,i_3}

$$\rho(\mathbf{r}) = \sum_{i_1,i_2,i_3} \rho_{i_1,i_2,i_3} \phi(x - i_1)\phi(x - i_2)\phi(x - i_3). \quad (1)$$

$$\sum_{i_1,i_2,i_3} i_1^{l_1} i_2^{l_2} i_3^{l_3} \rho_{i_1,i_2,i_3} = \int d\mathbf{r} x^{l_1} y^{l_2} z^{l_3} \rho(\mathbf{r}) \quad 0 \le l_1, l_2, l_3 < m. \quad (2)$$

19 m

$$M_l = \int \phi(x) x^l dx = \delta_l, \quad = 0, \ldots, m \quad 1. \quad (3)$$

$$\int \phi(x \quad j) x^l dx = \int \phi(t)(t - j)^l dt$$

$$= \int \phi(t) \sum_{p=0}^{l} C_l^p t^p j^{l \ p} dt = j^l$$

(1) (2)