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An $O(h^2)$ Coulomb singularity correction for the Bethe-Salpeter equation[1] DANIEL ABERG, BABAK SADIGH, ANDRE SCHLEIFE, TOMAS OPPELSTRUP, LLNL — We present an improved numerical correction, at no extra computational cost, for the Coulomb singularity in the Bethe Salpeter equation for bound excitonic states. This method leads to modifications of the off-diagonal matrix elements of the Bethe-Salpeter matrix with quadratic scaling of the asymptotic error. This method is particularly well suited for systems where hybrid Brillouin sampling schemes are ineffective, e.g., systems with an indirect fundamental band gap or large supercells containing defects. Numerical results are presented for the binding energy of the ground state excitons in the two-band model as well as the scintillator material CsI.

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