First Principles Calculation of Helical Spin Order in Iron Perovskite SrFeO$_3$ and BaFeO$_3$ ZHI LI, Yukawa Institute for Theoretical Physics, Kyoto University — Motivated by recent discovery of ferromagnetism in cubic perovskite BaFeO$_3$ under small magnetic field, we investigate spin order in BaFeO$_3$ and isostructural SrFeO$_3$ by a first principles calculation using local spin density approximation (LSDA). We find that on-site Coulomb interaction $U$ is necessary for obtaining helical spin order consistent with experiments. SrFeO$_3$ exhibits G-type helical order, while BaFeO$_3$ exhibits the A-type with very small wave vector. The A-type order is stabilized by lattice expansion. Small energy difference between the A-type and ferromagnetic orders explains ferromagnetism under small field. The LSDA+$U$ results are consistent with model calculation where negative charge-transfer energy in these compounds is explicitly taken into account.