



# Singular limit in the optimized effective potential with finite basis sets

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Most finite-basis set implementations of the optimized effective potential (OEP) method leave the potential undetermined, when the auxiliary basis set for the potential is sufficiently large. We discover that finite-basis OEP also exhibits previously unknown singular behaviour. We expect similar anomalous behaviour to be a general feature of single-particle theories where the response function, or the orbital Green's function, is truncated with a finite orbital basis set and then inverted. Imposing continuity, we derive new well-behaved finite-basis-set OEP equations that determine OEP for any auxiliary basis set and adopt an analytic solution via matrix-inversion.

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