Minimax Principle in Bivariational Functionals of Perturbation Theory

Michele Battezzati[a], Valerio Magnasco[b]

[a]via Bernardino Drovetti 7, 10138 Turin, Italy
[b]Dipartimento di Chimica e Chimica Industriale, via Dodecaneso 31, 16146 Genoa, Italy

Abstract

Use of double (or symmetry-adapted) perturbation theory in quantum mechanics requires evaluation of mixed matrix-elements of the Hamiltonian operator involving first-order perturbation functions. It was proved some time ago by us that a generalized Rayleigh-Ritz principle for these matrix elements holds, stating that the mixed matrix-element equals the sum of minimum and maximum values of an appropriate homogeneous functional $J[\chi]$ in Hilbert space of real square summable functions. The first-order solutions of perturbative equations then result as a quasi-linear combination of the extremizing functions.

The problem that is considered in this paper is that of reconstructing the first-order approximate solutions from the approximants to the solutions of the variational problem. It is proven that a solution to this problem may not exist upon requiring that the sum of approximate minimum and maximum values of $J[\chi]$ matches the value of the mixed matrix-element between the approximate first-order solutions. The required property necessitates an integral equation to be satisfied by the approximate extremizing functions.

It is shown that this condition can be met by suitable renormalization of the approximate perturbative solutions obtained from the free extrema of $J[\chi]$. The corresponding extremal points of the variational problem obtained from the inverse mapping, then, are not necessarily extrema, though their sum is expected to be stationary.

It is proven further that the first-order functions obtained by the proposed transformation satisfy authomatically an interesting homogeneous relation.

References

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