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ADDENDUM

Modification of the extended (2×2) algorithm by a variational principle

K G Kreuzer, H G Miller[†] and W A Berger[‡]

[†] Institut für Theoretische Physik, Universität Frankfurt, West Germany

[‡] Institut für Theoretische Physik, Universität Giessen, West Germany

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Abstract. The extended (2×2) algorithm is supplemented by a variational procedure which improves the convergence rate of the algorithm.

Recently we have demonstrated the applicability of the Lanczos and the (2×2) algorithm for obtaining the exact ground state of a full (unprojected) Hamiltonian of a quantum mechanical system (Kreuzer *et al* 1980a,b). Although in the case of the (2×2) algorithm each iteration step is essentially simpler, the rate of convergence is generally slower than that of the Lanczos algorithm, provided of course that the same initial trial state is used in both cases. This has already been demonstrated in the case of a finite-dimensional Hamiltonian matrix (Berger *et al* 1977), and is also valid in the case of the full Hamiltonian operator (Kreuzer 1978).

The convergence rate of the (2×2) algorithm may, however, be considerably improved by means of a simple variational procedure. In each iteration step one passes from the single trial state $|T\rangle$ to a family of trial states $|T(\beta)\rangle$ such that each member including $|T\rangle$ is specified by a definite value of the parameter β . Then the parameter is chosen in such a way that the expectation value of $|T(\beta)\rangle$ with the Hamiltonian \hat{H} becomes minimal with respect to β , i.e.

$$(d/d\beta)\langle T(\beta)|\hat{H}|T(\beta)\rangle = 0.$$

With the resulting trial state $|T(\beta_0)\rangle$, β_0 being the solution of the variational equation above, the (2×2) iteration step is then performed, yielding a vector $|e_1\rangle$, whose expectation value with \hat{H} is lower than that of $|T(\beta_0)\rangle$ (Kreuzer 1980b). The state $|e_1\rangle$ is then taken as a new trial state for restarting the procedure. Modifying the extended (2×2) algorithm in this manner yields the same final result as before, i.e. the ground state of the Hamiltonian but now with a much better convergence rate—provided of course that the usual requirements concerning the trial state are fulfilled (Kreuzer 1980b) and that in each iteration step the ground state is present in $|T(\beta)\rangle$ for each β . The convergence rate, as can be seen from the numerical example below, may be as good as that of the Lanczos algorithm. For the latter, such a modification is possible once at the most in the initial choice of the trial state, since otherwise the structure of the algorithm is destroyed.

As a numerical example we have calculated the ground state energy of the anharmonic oscillator in one dimension:

$$\left(-\frac{\hbar^2}{2m} \frac{d^2}{dx^2} + x^4\right) \langle x | E_0 \rangle = E_0 \langle x | E_0 \rangle$$

starting from a family of initial trial states given by

$$\langle x | T(\beta) \rangle := \alpha \exp(-\beta \gamma x^2 / 2).$$

Here α is a normalisation constant, $\gamma := (2m/\hbar^2)^{1/2}$ and β is a real parameter to be varied. The results are given in the two figures below. Figure 1 shows the convergence rates of the Lanczos algorithm and the (2×2) algorithm in the case where β was arbitrarily chosen. The convergence rates of the two algorithms obviously differ by a

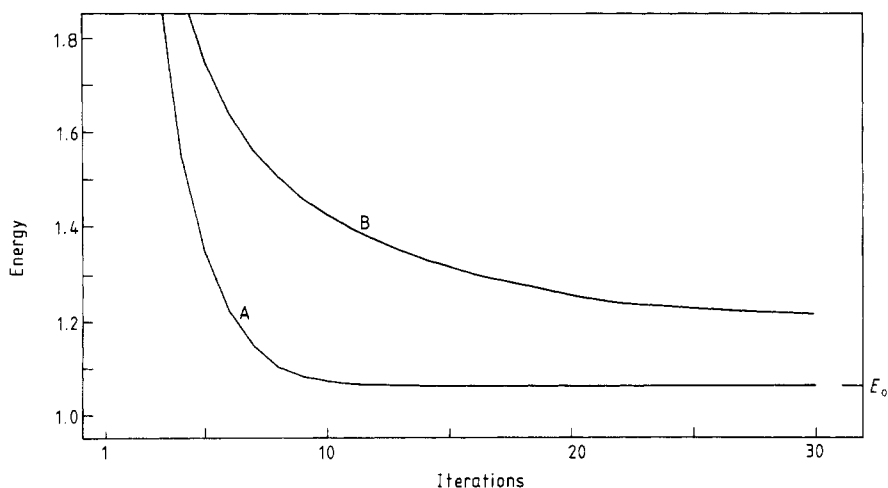


Figure 1. Convergence rate of the Lanczos algorithm (A) and the (2×2) algorithm (B) where in both cases $\beta = 10$. Units are chosen such that $\hbar^2/2m = 1$.

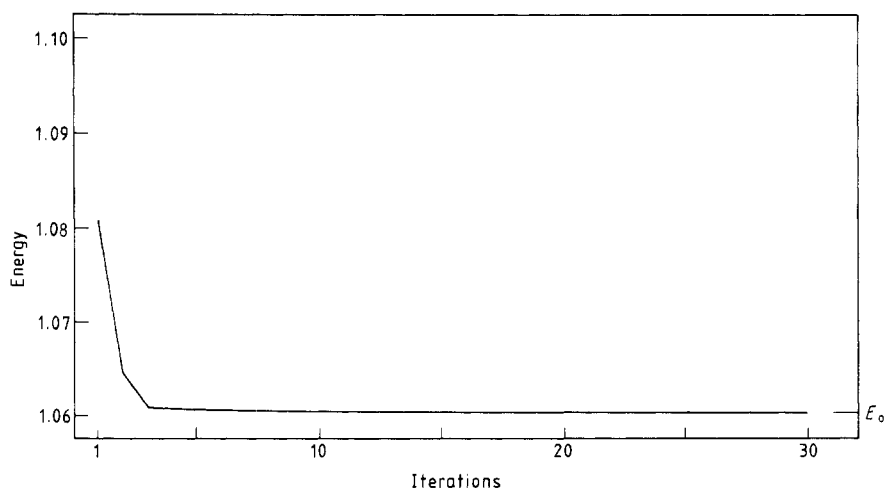


Figure 2. Convergence rate of the modified (2×2) algorithm.

considerable amount. Figure 2 shows the improvement of the convergence rate of the (2×2) algorithm when it is modified in the aforementioned manner. Choosing the initial trial state for the Lanczos algorithm such that $\langle T(\beta) | \hat{H} | T(\beta) \rangle$ is minimal, yields the same convergence rate within the numerical accuracy of the calculation.

The modification of the (2×2) algorithm in the manner outlined above is of course by no means restricted to a single variational parameter. It works as well in the case where one considers a family of trial states where each member is specified by several parameters. However, the variational equations in each iteration step become more extensive, but can be solved by standard techniques. Scaling the coordinates of the constituent particles of a quantum mechanical system (Löwdin 1959) should provide a simple means of passing from a single trial state to a family of trial states. In particular, in the case where the potential energy is a homogeneous function of the coordinates, the variation of the total energy expectation value with respect to the scaling parameters can be considerably simplified (Löwdin 1959).

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