Generation of Coulomb Matrix Elements for the 2D Quantum Harmonic Oscillator

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Extant analytic formulas [1] for evaluating electron-electron interaction matrix elements in Fock-Darwin basis suffer from numerical stability problems due to large cancellations in the range of medium to large values of the magnetic quantum numbers. The problem can be bypassed using symbolic calculus software but the computation time is often prohibitive in that regime.

The numerical reliability of an existing formula [1] and a novel expression presented in the poster are analyzed using computer-assisted algebraic techniques. We will show that our formula is clearly more stable but nevertheless, the analysis shows that the range of safety parameters is certainly narrow also, even using quadruple precision arithmetic.

The main contribution presented here involves a set of recurrence relations which make possible to compute the set of matrix elements by means of any algebraic software at a very high rate. The algorithm devised for using these recurrences is described in detail. Computation time comparison between a *Maple* implementation of our scheme and previous expressions [1] is presented, showing an overall improvement of two orders of magnitude. Finally we show that the algorithm is even faster than numerical evaluation in calculating all the matrix elements required when working with basis sets of practical size.

References

[1] P. Hawrylak, Solid State Communications **88** (1993) 475.