A low-scaling iterative algorithm for large-scale coupled-channel quantum scattering calculations

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Many interesting problems in molecular collision dynamics involve large systems of coupled-channel (CC) Schrödinger equations, which defy the computational state-of-the-art. A prominent example is given by ultracold Rb + KRb collisions, in which hyperfine-to-rotational energy transfer has recently been observed experimentally, driven by short-range spin-dependent interactions [1]. Rigorous quantum CC calculations on such collisions face enormous computational challenges due in part to the steep $O(N^3)$ scaling of current algorithms [2, 3] with the number of scattering channels N.

Here, we revisit a low-scaling [$O(N^2)$] iterative approach for calculating a single column of the S-matrix developed by Lowell Thomas [4, 5], which can potentially outperform the existing algorithms [2, 3] for large-scale CC computations. The approach is based on the iterative solution of the multichannel Lippmann-Schwinger equation, and is particularly well-suited for cold and ultracold collisions of molecules prepared in single quantum states.

We extend the original Thomas algorithm to include closed channels as necessary to obtain converged scattering observables, and apply it to cold He + CO collisions on an accurate *ab initio* potential energy surface. We obtain excellent agreement with benchmark CC results, highlighting the promise of the improved Thomas algorithm for solving large-scale quantum scattering problems.

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