

学术报告

Normalized gradient flow with Lagrange multiplier for computing ground states of Bose--Einstein condensates

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Abstract: The normalized gradient flow, i.e. the gradient flow with discrete normalization (GFDN) introduced in [W. Bao and Q. Du, SIAM J. Sci. Comput., 25 (2004), pp. 1674--1697] or the imaginary time evolution method is one of the most popular techniques for computing the ground states of Bose--Einstein condensates (BECs). In this talk, we revisit the time discretizations for the GFDN and its generalization to the multi-component BECs. Several widely used time discretizations are demonstrated not accurate for computing the ground state solution in the general case, especially for the multi-component BECs with two or more constraints even for the most accepted linearized backward Euler schemes. More precisely, these schemes usually converge to a solution with an error depending on the time step size. To accurately and efficiently compute the ground state solution of BECs, we propose the gradient flow with Lagrange multiplier (GFLM) method which can be viewed as the modified GFDN by introducing the explicit Lagrange multiplier terms or an approximation of the continuous normalized gradient flow (CNGF). Through analysis and numerical computation, we clarify that, in order to accurately compute the ground state solution, the GFDN method must be discretized in very special ways in time such as the linearized backward Euler scheme, while the GFLM can be discretized by various schemes and works for multi-component BEC with multiple constraints. We propose a simple backward-forward Euler scheme to discretize the GFLM, where only a linear system with constant coefficients needs to be solved at each time step. Taking the spin-1 BEC as an example, we demonstrate how traditional GFDN approach fails in computing the ground state solution of general multi-component BECs accurately. The proposed GFLM with backward-forward Euler discretization is shown to be accurate and efficient. Extensive numerical results are provided to verify our claims.

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