

Ground State of Nonlinear Schrödinger Equation as a Limit of a Gradient Flow

Jian-Guo Liu, University of Maryland

Fast computation of the ground state and excited states of nonlinear Schrödinger equation is important in many applications of physical problems such as Bose-Einstein condensation. Energy diminishing of a normalized gradient flow, also known as imaginary time method, is a typical method used in physical literature for computing the ground states. In this method, the solution procedure is alternating between time matching through a gradient flow and normalization. This numerical procedure is also known as projection method. The interruption of the normalization steps (projection steps) in the gradient flow usually slows down the convergence.

In the linear case, the normalization in the gradient flow corresponds to the Rayleigh quotient $E(u/\|u\|) = E(u)/\|u\|^2$. This quantity is found diminishing in the gradient flow. Indeed, it is true for a general nonlinear case with convex energy function. A new decay rate $\frac{d}{dt}E(u)/\|u\|^2 \leq -4\mathcal{E}(\mathcal{E} - E)/\|u\|^4$ is obtained for the general gradient flow. Here $E(u)$ and $\mathcal{E}(u)$ are energy and chemical potential, respectively.

As an application, we constructed a gradient flow such that its large time limit becomes the ground state of nonlinear Schrödinger equation. This gradient flow provides a fast numerical computation for the ground state. We also constructed a class of conservative Crank-Nicolson scheme which preserves this new decay rate estimate, as well as usual energy and normalization.