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Optimizing Schrödinger functionals using Sobolev gradients: Applications to quantum mechanics and nonlinear optics. (English) Zbl 0999.65058
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Summary: We study the application of the Sobolev gradients technique to the problem of minimizing several Schrödinger functionals related to timely and difficult nonlinear problems in quantum mechanics and nonlinear optics. We show that these gradients act as preconditioners over traditional choices of descent directions in minimization methods and show a computationally inexpensive way to obtain them using a discrete Fourier basis and a fast Fourier transform. We show that the Sobolev preconditioning provides a great convergence improvement over traditional techniques for finding solutions with minimal energy as well as stationary states and suggest a generalization of the method using arbitrary linear operators.

MSC:
- 65K10 Numerical optimization and variational techniques
- 78A15 Electron optics
- 82D50 Statistical mechanics of superfluids
- 78M50 Optimization problems in optics and electromagnetic theory
- 35Q55 NLS equations (nonlinear Schrödinger equations)
- 49J20 Existence theories for optimal control problems involving partial differential equations
- 81Q05 Closed and approximate solutions to the Schrödinger, Dirac, Klein-Gordon and other equations of quantum mechanics
- 49M15 Newton-type methods

Keywords:
- Sobolev gradients; ground states; nonlinear Schrödinger equations; quantum mechanics; nonlinear optics; discrete Fourier basis; fast Fourier transform; Sobolev preconditioning; convergence

Software:
- FFTW

Full Text: DOI arXiv