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A perturbation-method-based \textit{a posteriori} estimator for the planewave discretization of nonlinear Schrödinger equations

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Abstract

In this Note, we propose a new method, based on perturbation theory, to post-process the planewave approximation of the eigenmodes of periodic Schrödinger operators. We then use this post-processing to construct an accurate \textit{a posteriori} estimator for the approximations of the (nonlinear) Gross–Pitaevskii equation, valid at each step of a self-consistent procedure. This allows us to design an adaptive algorithm for solving the Gross–Pitaevskii equation, which automatically refines the discretization along the convergence of the iterative process, by means of adaptive stopping criteria.

Résumé

Dans cette Note, nous proposons une nouvelle méthode, basée sur la théorie des perturbations, pour post-traiter l'approximation dans une base d'ondes planes des modes propres d'opérateurs de Schrödinger périodiques. Nous utilisons ensuite ce post-traitement pour construire un estimateur d'erreur \textit{a posteriori} pour les approximations de l'équation de Gross–Pitaevskii (non-linéaire), valide à chaque étape de la procédure auto-cohérente. Ceci nous permet de proposer un algorithme adaptatif pour résoudre cette équation, qui raffine automatiquement la discrétisation au cours du processus itératif, par le biais de critères d'arrêt adaptatifs.

1. Introduction

The time-independent Gross–Pitaevskii and Kohn–Sham models are widely used in quantum physics to describe, respectively, steady states of Bose–Einstein condensates and electronic ground states of molecular systems. Although these models dramatically differ from the physical viewpoint (the former describes bosons, the latter describes fermions), their mathematical structures share some similarities: they are constrained optimization problems whose Euler–Lagrange equations are nonlinear elliptic eigenvalue problems. As a consequence, the numerical methods used to simulate these models have common features. In both cases, numerical solutions can be obtained either by minimization of the energy functional on the admissible set, or by solving the Euler–Lagrange equations by a self-consistent field (SCF) procedure. Algorithms mixing the two approaches have also been proposed.

Among the various discretization methods available, the planewave (Fourier) method is one of the most popular. It is in particular the state-of-the-art method for Kohn–Sham simulations in solid state...
We denote by \( \Pi_N \) setting corresponds to \( N \), where the Gross–Pitaevskii functional is given, in absence of an external magnetic field, by

\[
H_{\text{GP}}(v) := \int_{\Omega} \left( \frac{1}{2} |\nabla v|^2 + \mu |v|^2 + V(v) \right)
\]

where \( \mu > 0 \) and \( V \) is a real-valued, belongs to \( H^{s}_{\#}(\Omega) \) and compact resolvent. The variational approximation of (1) in the discretization space \( X_N \) gives rise to the finite-dimensional constrained optimization problem

\[
\inf \left\{ E_{\text{GP}}(v), \; v \in H^{s}_{\#}(\Omega), \; \|v\|_{L^2_\#} = 1 \right\},
\]

(2)

As \( \Pi_N \) and the Laplace operator commute, the minimizer \( \lambda_N \) of (2) satisfies

\[
-\Delta u_N + \Pi_N \left( (V + |u_N|^2) u_N \right) = \lambda_N u_N, \quad \|u_N\|_{L^2_\#} = 1,
\]

(3)

where \( \lambda_N \) is the Lagrange multiplier associated with the constraint \( \|u_N\|_{L^2_\#} = 1 \). It is proved in [2] that, for \( N \) large enough, the discretized problem (2) has a unique real-valued minimizer \( u_N \) such that
(u, u_N)_{L^2_\mu} \geq 0 \text{ (the other minimizers being equal to } u_N \text{ up to a global phase), and that the following optimal } a \text{ priori error estimates hold}

c \|u - u_N\|^2_{H^2_\mu} \leq E(u_N) - E(u) \leq C \|u - u_N\|^2_{H^1_\mu}, \quad |\lambda - \lambda_N| \leq C N^{-2(s+1)}, \quad \|u - u_N\|_{H^s_\mu} \leq C N^{-(s+2-r)},

(4)

for all \(-s \leq r < s + 2\), and where the constants \(c\) and \(C\) depend on \(\|V\|_{H^s_\mu}\) and \(\mu\) but are independent of \(N\).

As mentioned above, the discretized problem (3) can be solved either by constrained minimization or by SCF algorithms. Our approach can be applied to a variety of iteration schemes, but for brevity, we only discuss here the simple case of the Roothaan algorithm. We are aware that the Roothaan algorithm is far from being the most efficient algorithm to solve the Gross–Pitaevskii equation, but we nevertheless chose it for two reasons: first, it allows us to illustrate our approach on a simple example where technicalities are reduced to a minimum, and second this algorithm is somewhat similar to the SCF algorithms actually used in Kohn–Sham simulations.

The purpose of this Note is twofold. First, we propose a method to post-process the planewave approximation of the eigenmodes of (linear) periodic Schrödinger operators and obtain a much better accuracy for a limited extra computational cost. This post-processing, although based on a simple application of the perturbation method, seems to be new. Note that this approach can be extended to the case of the (nonlinear) Gross-Pitaevski equation [3]. Second, we use this post-processing to construct an accurate \(a\) posteriori error estimator for the Gross–Pitaevskii equation. This estimator allows us to design an adaptive algorithm for solving this equation, which automatically refines the discretization along the convergence of the SCF iterations, by means of adaptive stopping criteria. The first steps of the SCF procedure are carried out in a coarse discretization space (it is indeed a loss of time to use a fine discretization space far from the minimizer), and the cut-off \(N\) is gradually increased to balance the two components of the total error: the discretization error on the one hand, and the error due to the fact that the SCF iterations has not converged yet on the other hand. The extension of this approach to more complex nonlinear Schrödinger equations and to the Kohn–Sham model is work in progress.

2. Post-processing of the planewave approximation of periodic Schrödinger operators

We first consider a generic linear periodic Schrödinger operator \(H = -\Delta + W\) on \(L^2_\mu(\Omega)\), with \(W \in H^s_\mu(\Omega)\) for some \(s \geq 0\). In regard of the previous section, \(H\) can denote the linearized Gross–Pitaevskii Hamiltonian \(H_{w^{j-1}} = -\Delta + V + \mu(w^{j-1})^2\) at step \(j\) around an approximation \(w^{j-1}\) for example. For simplicity, we focus on the ground state eigenvalue \(\nu\) of \(H\), but our argument straightforwardly extends to any non-degenerate eigenvalues by using the minmax principle. The case of degenerate eigenvalue is dealt with in [3]. Denoting by \(w \in H^s_\mu(\Omega)\) the unique positive ground state of \(H\), it is well-known that the optimization problem

\[
\nu_N = \inf \left\{ E_2(v_N), \ v_N \in X_N, \ \|v_N\|_{L^2_\mu} = 1 \right\} \quad \text{with} \quad E_2(v) := \int_\Omega |\nabla v|^2 + \int_\Omega |Wv|^2 = (v, Hv)_{L^2_\mu}
\]

has a unique real-valued minimizer \(w_N\) such that \((w_N, 1)_{L^2_\mu} \geq 0\), and that (focusing on the \(H^1\)-norm for brevity)

\[
c \|w - w_N\|^2_{H^1_\mu} \leq \nu_N - \nu \leq C \|w - w_N\|^2_{H^1_\mu} \quad \text{and} \quad \|w - w_N\|_{H^1_\mu} \leq C N^{-(s+1)},
\]

with \(0 < c \leq C < \infty\) constants independent of \(N\). The observation our approach is based upon is that \((\nu_N, w_N)\) satisfies
\[
H_Nw_N = \nu_Nw_N, \quad ||w_N||_{L^2_\omega}^2 = 1 \quad \text{where} \quad H_N = -\Delta + \Pi_NW\Pi_N,
\]
while \((\nu, w)\) satisfies
\[
(H_N + W_N)w = \nu w, \quad ||w||_{L^2_\omega}^2 = 1 \quad \text{with} \quad W_N = \Pi_N^1W\Pi_N + \Pi_N^2W\Pi_N^1 + \Pi_N^3W\Pi_N^2.
\]
In addition, it can be seen that as soon as \(N^2 > \nu_N\), \(w_N\) is the ground state of \(H_N\). It therefore makes sense to apply Kato’s perturbation theory using \((\nu_N, w_N)\) as the reference solution and \((\nu, w)\) as the perturbed solution, in order to build improved approximations \((\tilde{\nu}_N, \tilde{w}_N)\) based upon perturbation arguments. A simple calculation shows that the first order correction to the eigenfunction \(w_N\) is given by
\[
w^{(1)}_N = (-\Delta|_{X_N^\perp} - \nu_N)^{-1}r_N \quad \text{where} \quad r_N = Hw_N - \nu_Nw_N = \Pi_N^1(Ww_N) \in X_N^\perp
\]
is the residual of the eigenvalue problem. The first order correction to the eigenvalue vanishes and the second order correction is (using Dirac’s bra-ket notation)
\[
\nu^{(2)}_N = (w^{(1)}_N, r_N)_{L^2_\omega} = -\langle r_N | (-\Delta|_{X_N^\perp} - \nu_N)^{-1}r_N \rangle.
\]
Note that \(w^{(1)}_N\) and \(\nu^{(2)}_N\) are well-defined (provided that \(N^2 > \nu_N\)) and computable by a single Fast Fourier Transform on a finer grid. An extension to the result below to more general operators and discretization spaces, higher-order perturbations, and degenerate eigenvalues, is proved in [3].

**Lemma 2.1 ([3])** \(\) Let \(W \in H^s_\#(\Omega)\) for some \(s > d/2\). For all \(N \in \mathbb{N}\) such that \(N^2 > \nu_N\), the quantities \(\tilde{w}_N = w_N + w^{(1)}_N\) and \(\tilde{\nu}_N = \nu_N + \nu^{(2)}_N\) are well-defined and there exists a constant \(C > 0\) independent of \(N\) such that
\[
|\nu - \tilde{\nu}_N| \leq CN^{-2}|\nu - \nu_N| \quad \text{and} \quad ||w - \tilde{w}_N||_{H^1_\omega} \leq CN^{-2}||w - w_N||_{H^1_\omega}.
\]

**3. A posteriori estimators and adaptive algorithms for the Gross–Pitaevskii equation**

We now use the results established in the previous section to design an adaptive algorithm based on the Roothaan procedure for the solution of (3), whose iterations are defined by:
\[
-\Delta u^j + \Pi_{N_j}(Vu^j + \mu|u^{j-1}|^2u^j) = \lambda^j u^j, \quad u^j \in X_{N_j}, \quad ||u^j||_{L^2_\omega}^2 = 1, \quad (u^j, 1)_{L^2_\omega} \geq 0, \quad (5)
\]
where \(u^0 \in X_{N_0}\) is a given initial guess, and where \((N_j)_{j \in \mathbb{N}}\) is a non-decreasing sequence of integers. Note that \(u^j\) is in some sense a shortcut notation for \(u^j_{N_j}\), since this function belongs to the discrete space \(X_{N_j}\). Usually, \(N_j\) is kept constant (equal to \(N\)) along the iterations. In our approach, the sequence \((N_j)_{j \in \mathbb{N}}\) is not specified a priori, but automatically constructed by the algorithm. This is achieved by using an a posteriori estimator of the error between \(u^j\) and \(u\), which can be decomposed into two non-negative contributions:

i) a contribution \(\eta_{\text{scf}}^j\) measuring the error at step \(j\) due to the fact that the SCF procedure has not converged;

ii) a contribution \(\eta_{\text{dis}}^j\) measuring the error at step \(j\) due to the fact that \(u^j\) is a finite-dimensional approximation of \(u\) in \(X_{N_j}\).

Following the ideas of [1,4,5], we propose to refine the discretization space whenever \(\eta_{\text{scf}}^j \leq \zeta \eta_{\text{dis}}^j\), where \(\zeta\) is some user-given parameter, typically of order 0.1. The new discretization parameter \(N_{j+1}\) can then be chosen by linear regression based on the a priori convergence rate in order that the predicted new discretization error is smaller than \(\zeta'\eta_{\text{scf}}^j\) for some user-given parameter \(\zeta'\).
Let us now provide explicit expressions for $\eta^j_{\text{act}}$ and $\eta^j_{\text{dis}}$. As usual in a posteriori error estimations, we begin with discussing the choice of the measure of the error. A common choice for nonlinear problems is the energy difference $E_{\text{GP}}(u^j) - E_{\text{GP}}(u)$. In our setting, it appears that we can better estimate the augmented energy difference $J_u(v^j)$ where

$$J_u(v^j) := E_{\text{GP}}(v^j) - E_{\text{GP}}(u) + \frac{H}{2} \int_\Omega (|u|^2 - |v|^2)^2.$$ 

Note that for all $v \in H^1_#(\Omega)$ such that $\|v\|_{L^2_\#} = 1$ and $(v, 1)_{L^2_\#} \geq 0$, $J(v) \geq 0$ and $J(v) = 0$ if and only if $v = u$. We also know from \cite{1} that there exists $0 < c \leq C < \infty$ such that $c \|v - u\|^2_{H^1_\#} \leq J_u(v) \leq C \|v - u\|^2_{H^1_\#}$ for all $v \in H^1_#(\Omega)$ such that $\|v\|_{L^2_\#} = 1$ and $(v, 1)_{L^2_\#} \geq 0$.

**Theorem 3.1** (\cite{3}) Let $u$ be the exact solution of (1) satisfying $u > 0$ in $\Omega$ and $w^j \in X_{N_j}$ the numerical approximation of $u$ generated by the iterative procedure (5) at step $j$. Then

$$J_u(v^j) \leq \eta^j_{\text{tot}} := \left( \lambda^j - \lambda^{j+1}_{\text{db}} + \int_\Omega [(w^j)^2 - (u^{j-1})^2]|(w^j)^2 \right),$$

where $\lambda^{j+1}_{\text{db}}$ is a lower bound of the exact ground state eigenvalue $\lambda^{j+1}_{\text{infty}}$ of $H_{\text{db}}$. In addition, the error bound $\eta^j_{\text{tot}}$ can be decomposed as $\eta^j_{\text{tot}} = \eta^j_{\text{act}} + \eta^j_{\text{dis}}$ where

$$\eta^j_{\text{dis}} := \left( \lambda^{j+1}_{N_j} - \lambda^{j+1}_{\text{db}} \right) \geq 0, \quad \eta^j_{\text{act}} := \left( \int_\Omega [(w^j)^2 - (u^{j-1})^2](w^j)^2 + \lambda^j - \lambda^{j+1}_{N_j} \right) \geq 0,$$

where $\lambda^{j+1}_{N_j}$ is the variational approximation of $\lambda^{j+1}_{\text{infty}}$ in the discretization space $X_{N_j}$.

In the numerical results reported in the next section, we first compute $\lambda^{j+1}_{\text{db}}$ as the lowest eigenvalue of $-\Delta + \Pi_{N_j} W \Pi_{N_j}$ with $W = V + \mu |u|^2$ (which amounts to make one more iteration of the Roothaan algorithm in the discretization space $X_{N_j}$), and we estimate $\lambda^{j+1}_{\text{infty}}$ by post-processing $\lambda^{j+1}_{N_j}$ thanks to the perturbation argument provided in Section 2. Although the so-obtained post-processed eigenvalue is not strictly speaking a lower bound of $\lambda^{j+1}_{\text{infty}}$, it is an excellent approximation of it and can be therefore be used instead of $\lambda^{j+1}_{\text{db}}$ to compute the error estimators in Theorem 3.1. Note that it is also possible to use perturbation theory to estimate both $\lambda^{j+1}_{N_j}$ and $\lambda^{j+1}_{\text{db}}$ (see \cite{3}).

4. Numerical Results

We first consider the linear one-dimensional periodic Schrödinger operator with potential $W(x) = |\sin(2\pi x)| + 6$ and $\Omega = (0, 1)$. We observe in Fig. 1 (left) very good agreements with the theoretical results of Lemma 2.1. We then report in Fig. 1 (right) simulations of the one-dimensional Gross–Pitaevskii equation with $V(x) = |\sin(2\pi x)| + 6$ and $\mu = 1$, showing the decay of different quantities related to Theorem 3.1 for a fixed $N = 50$ during the Roothaan iterations, and illustrating the sharpness of the estimator and the splitting of the error components. More extensive numerical results in higher dimensions will be presented in \cite{3}.

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Figure 1. Left: Convergence rate with respect to $N$ with and without post-processing the eigenvector as well as the quotient $q_N = \|w - \tilde{w}_N\|_{H^1_0}/\|w - w_N\|_{H^1_0}$. Right: Convergence of the error in the energy and the augmented energy difference $J_u(w')$, and a posteriori estimators with respect to the Roothaan iterations for $N = 50$. Gauche : Taux de convergence par rapport à $N$ avec et sans post-traitement du vecteur propre et quotient $q_N = \|w - \tilde{w}_N\|_{H^1_0}/\|w - w_N\|_{H^1_0}$. Droite : Convergence de l’erreur sur l’énergie et la différence d’énergie augmentée $J_u(w')$, et estimateurs a posteriori en fonction des itérations de Roothaan pour $N = 50$.

References