A priori analysis of Schrödinger equations with analytic potentials

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This talk is concerned with the numerical analysis of linear and nonlinear Schrödinger equations with analytic potentials. We introduce a hierarchy $(\mathcal{H}_A)_{A>0}$ of function spaces of complex-valued 2π-periodic functions on the real line which admit analytic extensions on a horizontal strip of width $2A$ of the complex plane. We then consider a real-valued function $V \in \mathcal{H}_B$ for some $B > 0$, and the corresponding Schrödinger operator $H = -\Delta + V$ acting on the Hilbert space $L^2_{\rm per}$ of complex-valued 2π-periodic functions on $\mathbb{R}$.

We study the $\mathcal{H}_A$ regularity of the solutions to (i) the linear problem $Hu = f$ for a given $f \in \mathcal{H}_A$, (ii) the linear elliptic eigenvalue problem $Hu = \lambda u$, and (iii) the nonlinear elliptic eigenvalue problem $Hu+\mu u^3 = \lambda u$. We also study the rate of convergence of the planewave (Fourier) discretization method for computing numerical approximations of u. While the regularity of V (and f) automatically conveys to u in the linear case (in the sense that e.g. the eigenfunctions of H are in $\mathcal{H}_A$ for all $0 < A < B$), this is no longer true in general in the nonlinear case. Our results, which can be easily extended to the multidimensional case, are motivated by the numerical analysis of Kohn-Sham density functional theory with entire pseudopotentials such as the ones introduced by Goedecker, Teter, and Hutter, and used in the DFTK software [1].

[1] M. F. Herbst, A. Levitt, E. Cancès. *DFTK : A Julian approach for simulating electrons in solids.* Proc. JuliaCon Conf., **3**, 69, 2021. doi :10.21105/jcon.00069.

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