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Continuum Limit for Discrete NLS with Memory Effect

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Abstract We consider a discrete nonlinear Schrödinger equation with long-range interactions and a memory effect on the infinite lattice $h\mathbb{Z}$ with mesh-size $h > 0$. Such models are common in the study of charge and energy transport in biomolecules. Because the distance between base pairs is small, we consider the continuum limit: a sharp approximation of the system as $h \to 0$. In this limit, we prove that solutions to this discrete equation converge strongly in L^2 to the solution to a continuous NLS-type equation with a memory effect, and we compute the precise rate of convergence. In order to obtain these results, we generalize some recent ideas proposed by Hong and Yang in L^2-based spaces to classical functional settings in dispersive PDEs involving the smoothing effect and maximal function estimates, as originally introduced in the pioneering works of Kenig, Ponce and Vega. We believe that our approach may therefore be adapted to tackle continuum limits of more general dispersive equations.

Keywords Continuum limit, NLS, memory effect

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1. Introduction

1.1. Background

The study of nonlinear dispersive equations on lattices is of fundamental importance to model charge and energy transport in biomolecules [26]. From computational and analytical perspectives, the analysis of such equations is quite challenging given their size and mathematical complexity. One way to simplify this analysis is by exploiting two aspects of such models: the large number of base pairs in these biomolecules and the small distance between them. In particular, one typically considers an infinite lattice of equispaced base pairs with mesh size $h > 0$ and considers the limit as $h \to 0$. This continuum limit can often be shown to solve a simpler (continuous) PDE which captures the main aspects of the discrete system.

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One of the most common models in biological physics is the following:

$$\begin{cases} i\partial_t u_h(t,x_m) = h\sum_{n\neq m} J_{n-m}\left[u_h(t,x_n) - u_h(t,x_m)\right] \pm |u_h(t,x_m)|^2 u_h(t,x_m), \\ u_h|_{t=0} = f_h. \end{cases} \tag{1.1}$$

where $u_h : [0,T]\times h\mathbb{Z} \to \mathbb{C}$ is the wave function, and where $x_m = hm \in h\mathbb{Z}$ live in the one-dimensional lattice with mesh size $h > 0$. The cubic nonlinearity represents a four-wave interaction, where a $+$ sign corresponds to a repulsive on-site self-interaction, and $-$ corresponds to the focusing case. One often assumes that the initial distribution f_h is the discretization of some continuous function $f : \mathbb{R} \to \mathbb{C}$, which is defined as follows:

$$f_h(x_m) = \frac{1}{h}\int_{x_m}^{x_{m+1}} f(x)\,\mathrm{d}x \qquad \text{for } m \in \mathbb{Z}. \tag{1.2}$$

The interactions between different base pairs are modelled by the kernel $\{J_n\}_{n\in\mathbb{Z}}$. A typical modeling choice [26] is a law that is inversely proportional to some power of the distance between them:

$$J_{m-n} := |x_m - x_n|^{-1-\alpha} \quad \text{for } m \neq n \in \mathbb{Z}, \quad \alpha > 0. \tag{1.3}$$

The model (1.1) was first studied by Kirkpatrick, Lenzmann and Staffilani in the context of quantum mechanics [22]. The main goal is to derive a continuum limit, i.e. to obtain a simpler continuous model that approximates the dynamics of the discrete model (1.1) as the distance between base pairs h tends to zero. Such continuum limits have been proved in the context of the NLS equation with a discrete Laplacian [6, 17], the NLS equation on a large but finite lattice [16], fractional NLS in 2D [7], dispersion-managed nonlinear NLS [8], the Ablowitz-Ladik system [21], the Klein-Gordon equation [5], and others.

In [22], Kirkpatrick, Lenzmann and Staffilani show that under mild technical conditions, the asymptotic behavior of the interactions (1.3) is all that matters. In other words, if

$$\lim_{n\to\infty} |x_n|^{1+\alpha} J_n = C_\alpha > 0, \tag{1.4}$$

for $\alpha \in (1,2)$, then the continuum limit of the solution to (1.1) (as $h \to 0$) is the solution to the fractional cubic NLS equation:

$$\begin{cases} i\,\partial_t u = c_\alpha\,(-\Delta)^{\frac{\alpha}{2}} u \pm |u|^2 u, \quad x \in \mathbb{R}, \\ u|_{t=0} = f. \end{cases} \tag{1.5}$$

A choice of $\alpha \in (1,2)$ is common in order to model long-range interactions between base pairs, see [26]. It is interesting to mention that when $\alpha \geq 2$, the interactions decay so fast that only local effects survive in the continuum limit. In this case, the continuum limit is the solution to the cubic NLS equation with the usual Laplacian (but note that condition 1.4 must be slightly modified).

Unfortunately, there are some limitations to these results. From a mathematical viewpoint, the regularity of the initial discrete distribution f_h in (1.1) is rather high compared to the continuous theory for NLS equations. This is due to the use of the Sobolev embedding in the proof of local well-posedness of the discrete equation.