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In the present Letter we use the Wannier function basis to construct lattice approximations of the nonlinear Schrödinger equation with a periodic potential. We show that the nonlinear Schrödinger equation with a periodic potential is equivalent to a vector lattice with long-range interactions. For the case-example of the cosine potential we study the validity of the so-called tight-binding approximation i.e., the approximation when nearest neighbor interactions are dominant. The results are relevant to Bose-Einstein condensate theory as well as to other physical systems like, for example, electromagnetic wave propagation in nonlinear photonic crystals.
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Interplay between nonlinearity and periodicity is the focus of numerous recent studies in different branches of modern physics. The theory of Bose-Einstein condensates (BEC) within the framework of the mean field approximation [1] is one of them. Recent interest in the effects of periodicity in BEC's has been stimulated by a series of remarkable experiments realized with BEC's placed in a potential created by a laser field [2] (the so-called *optical lattice*). Nonlinearity and periodicity have been observed to introduce fundamental changes in the properties of the system. On the one hand periodicity modifies the spectrum of the underlying linear system resulting in the potential of existence of new coherent structures, which could not exist in a homogeneous nonlinear system. On the other hand, nonlinearity renders accumulation and transmission of energy possible in "linearly" forbidden frequency domains; this, in turn, results in field localization. This situation is fairly general and can be found in other applications, such as the theory of electromagnetic wave propagation in periodic media (so-called photonic crystals) [3].

The study of nonlinear evolution equations with periodic coefficients is a challenging and interdisciplinary problem. This problem cannot be solved exactly in the general case and thus gives rise to various approximate approaches. One of them, borrowed from the theory of solid state [4], is the reduction of a continuous evolution problem to a lattice problem (i.e., reduction of a partial differential equation to a differential-difference one). It turns out that the relation between the properties of periodic and discrete problems is indeed rather deep (for a recent discussion of the relevant connections see e.g., [5] and references therein). Following the solid state terminology here we will refer to a discrete approximation when only nearest neighbor interactions are taken into account as a *tight-binding model*. This model has recently been employed in the description of BEC in an optical lattice [6]. One of the advantages of the lattice approach is that it allows one to obtain strongly localized configurations, the so-called *intrinsic localized modes* (ILM) (also called *breathers*) [7], in a rather simple way. These entities correspond to *gap solitons* of the original continuum model. In the above mentioned works a formal analysis has been provided, using a basis of functions strongly localized about the minima of the periodic potential. This basis, however, has not been presented explicitly and even its existence has not been established.

In this work we propose to use Wannier-function (WF) [4,8] as a complete set of functions localized near the minima of the potential, to reduce the evolution of a nonlinear partial differential equation with periodic coefficients to a nonlinear lattice. WF has recently been used both in connection with BEC in optical lattices [9] and in connection to gap solitons in nonlinear photonic crystals [10]. In our case this approach leads to *a vector set* of lattice equations. These lattice equations *exactly* correspond to the original continuum problem and the scalar tight-binding approximation can be deduced from them under some specific conditions. Checking these conditions one can analyse the applicability of the tight-binding model. In particular, we argue that although the ILM's reported in [6] do exist, their dynamics and stability must be studied within the framework of a more general vector-lattice equation.

Being interested in BEC applications we base our analysis on the ubiquitous example of the nonlinear Schrödinger equation

$$i\frac{\partial \psi}{\partial t} = -\frac{\partial^2 \psi}{\partial x^2} + V(x)\psi + \sigma|\psi|^2\psi \qquad (1)$$

where $\sigma = \pm 1$ and $V(x)$ is a periodic potential $V(x+L) =$

$V(x)$ [14]. Consider the eigenvalue problem associated with (1)

$$-\frac{d^2\varphi_{k,\alpha}}{dx^2} + V(x)\varphi_{k,\alpha} = E_\alpha(k)\varphi_{k,\alpha} \qquad (2)$$

where $\varphi_{k,\alpha}$ has Bloch (Floquet) functions (BF's) $\varphi_{k,\alpha} = e^{ikx}u_{k,\alpha}(x)$, with $u_{k,\alpha}(x)$ periodic with period L, and α is an index which labels energy bands $E_\alpha(k)$. As is well known, [4,8] $E_\alpha(k+\frac{2\pi}{L}) = E_\alpha(k)$; thus one can represent the energy as a Fourier series

$$E_\alpha(k) = \sum_n \hat{\omega}_{n,\alpha}\, e^{iknL}, \qquad \hat{\omega}_{n,\alpha} = \hat{\omega}_{-n,\alpha} = \hat{\omega}_{n\alpha}^* \quad (3)$$

where an asterisk stands for complex conjugation and

$$\hat{\omega}_{n,\alpha} = \frac{L}{2\pi}\int_{-\pi/L}^{\pi/L} E_\alpha(k)e^{-iknL}dk\,. \qquad (4)$$

The BF's constitute an orthogonal basis. However, for our purposes it is more convenient to use the WF's instead of the BF's. We recall that the WF centered around the position nL (n is an integer) and corresponding to the band α is defined as

$$w_\alpha(x-nL) = \sqrt{\frac{L}{2\pi}}\int_{-\pi/L}^{\pi/L}\varphi_{k,\alpha}(x)e^{-inkL}dk. \qquad (5)$$

Conversely,

$$\varphi_{k,\alpha}(x) = \sqrt{\frac{L}{2\pi}}\sum_{n=-\infty}^{\infty} w_{n,\alpha}(x)e^{inkL}. \qquad (6)$$

Similarly to BF's, they form a complete orthonormal (with respect to both n and α) set of functions, which, by properly choosing the phase of the BF's in (5), can be made real and exponentially decaying at infinity [8]. In what follows we assume that this choice is made: $w_{n,\alpha}^*(x) = w_{n,\alpha}(x)$. Due to completeness of WF's, any solution of (1) can be expressed in the form

$$\psi(x,t) = \sum_{n\alpha} c_{n,\alpha}(t)w_{n,\alpha}(x) \qquad (7)$$

which after substitution in (1) gives

$$i\frac{dc_{n,\alpha}}{dt} = \sum_{n_1} c_{n_1,\alpha}\hat{\omega}_{n-n_1,\alpha} +$$
$$\sigma\sum_{\alpha_1,\alpha_2,\alpha_3}\sum_{n_1,n_2,n_3} c_{n_1,\alpha_1}^* c_{n_2,\alpha_2} c_{n_3,\alpha_3} W_{\alpha\alpha_1\alpha_2\alpha_3}^{nn_1n_2n_3} \quad (8)$$

where

$$W_{\alpha\alpha_1\alpha_2\alpha_3}^{nn_1n_2n_3} = \int_{-\infty}^{\infty} w_{n,\alpha}w_{n_1,\alpha_1}w_{n_2,\alpha_2}w_{n_3,\alpha_3}dx \qquad (9)$$

are overlapping matrix elements. Since WF's are real, $W_{\alpha_1\alpha_2\alpha_3\alpha_4}^{n_1n_2n_3n_4}$ is symmetric with respect to all permutations within the groups of indices $(\alpha,\alpha_1,\alpha_2,\alpha_3)$ and

(n,n_1,n_2,n_3). Eq. (8) can be viewed as a vector discrete nonlinear Schrödinger (DNLS) equation for $\mathbf{c}_n =\mathrm{col}(c_{n1},c_{n2},...)$ with long-range interactions. In its general form, Eq. (8) is not solvable; however it allows reductions to simpler lattices in a number of important special cases. Below we list some of them.

(i) If the coefficients of the Fourier series (3) decay rapidly and $|\hat{\omega}_{1,\alpha}| \gg |\hat{\omega}_{n,\alpha}|$, $n > 1$ one can neglect long-range interaction terms in the linear part of Eq. (8) taking into account nearest neighbors only.

(ii) Since $w_{n,\alpha}(x)$ is localized and centered around $x = nL$, one can assume that in some cases among all the coefficients $W_{\alpha\alpha_1\alpha_2\alpha_3}^{nn_1n_2n_3}$ those with $n = n_1 = n_2 = n_3$ are dominant and other terms can be neglected. Then, taking into account points (i), (ii) one arrives at the equation

$$i\frac{dc_{n,\alpha}}{dt} = \hat{\omega}_{0,\alpha}c_{n,\alpha} + \hat{\omega}_{1,\alpha}(c_{n-1,\alpha} + c_{n+1,\alpha}) +$$
$$+\sigma\sum_{\alpha_1,\alpha_2,\alpha_3} W_{\alpha\alpha_1\alpha_2\alpha_3}^{nnnn}c_{n,\alpha_1}^* c_{n,\alpha_2}c_{n,\alpha_3} \qquad (10)$$

which degenerates into the tight-binding model [6]

$$i\frac{dc_{n,\alpha}}{dt} = \hat{\omega}_{0,\alpha}c_{n,\alpha} + \hat{\omega}_{1,\alpha}(c_{n-1,\alpha} + c_{n+1,\alpha})$$
$$+\sigma W_{1111}^{nnnn}|c_{n,\alpha}|^2 c_{n,\alpha} \qquad (11)$$

if one restricts consideration to the band α only. Note that within the single band approximation, Eq. (11) can be generalized by including next nearest neighbor overlapping terms from Eq. 8, thus leading to the mixing of on-site and intra-site nonlinearities of the same type as in the model introduced in [11]. It should also be mentioned that the coefficients $W_{\alpha\alpha_1\alpha_2\alpha_3}^{nnnn}$ in Eq. (10) are *independent* of n.

(iii) In the general case, however, single band descriptions can become inadequate (see below) due to resonant interband interactions induced by nonlinearity (this is quite different from *linear* solid state physics where interband transitions are usually induced by external forces). In this case Eq. (10) can be further simplified by supposing that the periodic potential depends on some parameter ϵ: $V(x) \equiv V_\epsilon(x)$, such that $\hat{\omega}_{1,\alpha} \equiv \hat{\omega}_{1,\alpha}(\epsilon) = O(\epsilon)$ when $\epsilon \to 0$. After the transformation $c_{n,\alpha}(t) = \exp\{i\hat{\omega}_{0,\alpha}t\}\tilde{c}_{n,\alpha}(t)$ one arrives at the equation for $\tilde{c}_{n,\alpha}$ with explicit dependence on t in the nonlinear terms in the form of oscillating exponents $\exp[i(\hat{\omega}_{0,\alpha} + \hat{\omega}_{0,\alpha_1} - \hat{\omega}_{0,\alpha_2} - \hat{\omega}_{0,\alpha_3})t]$. Let also $\tilde{c}_{n,\alpha}(0)$ be small enough. Then on the timescale $1/\epsilon$ these exponents are rapidly oscillating unless $\alpha = \alpha_2, \alpha_1 = \alpha_3$ or $\alpha = \alpha_3, \alpha_1 = \alpha_2$ Then, denoting $W_{\alpha\alpha_1\alpha\alpha_1}^{nnnn} \equiv W_{\alpha\alpha_1}$ (the coefficients $W_{\alpha\alpha_1}$ do not depend on n and describes interband interactions), and using time averaging techniques [13], one can reduce the lattice equation (10) to the form

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$$i\frac{d\tilde{c}_{n,\alpha}}{dt} = \hat{\omega}_{1,\alpha}(\tilde{c}_{n-1,\alpha} + \tilde{c}_{n+1,\alpha}) +$$
$$+ \sigma \sum_{\alpha_1} W_{\alpha\alpha_1}|\tilde{c}_{n,\alpha_1}|^2 \tilde{c}_{n,\alpha}. \quad (12)$$

This is a vector DNLS equation with coupling between bands of the cross phase modulation type [15]. To investigate ILM solutions in the Wannier representation we can restrict to the scalar case described by Eq. (11) for which construction of ILM's is well-established [7]. ILM's with multiple components of $\tilde{c}_{n,\alpha}$ populated can also be constructed (see below).

Several comments about the above assumptions are in order. Firstly, the latter imply that the procedure of reduction of the NLS with periodic coefficients to a lattice is a multistep process, and thus different lattices will appear for different regions of the parameters. Secondly, for the reduction to be consistent, the parameters of the problem must provide us with a small parameter. Thus the largest of the quantities $\hat{\omega}_{n,\alpha}/\hat{\omega}_{1,\alpha}$ $(n > 1)$ and $W_{\alpha\alpha_1\alpha_2\alpha_3}^{nn_1n_2n_3}/W_{\alpha\alpha_1\alpha_2\alpha_3}^{nnnn}$ $(n_j \neq n)$ will define this small parameter of the problem. This, in particular, means that simplification of the lattice equation, and hence the reasoning for the reduction to a lattice model, are (potentially) not always available for all parametric regimes, and must be verified for each model.

In the present Letter we study the validity of the above assumptions for Eq. (1) with the potential $V(x) = A\cos(2x)$ (which corresponds to the typical experimental setting for BEC in optical lattices [2]). In this case Eq. (2) is the Mathieu equation. Table I shows the coefficients $\hat{\omega}_{n,\alpha}$ for the three lowest energy bands for $A = -1$ and $A = -15$.

	$A = -1$			$A = -15$		
n	$\alpha = 1$	$\alpha = 2$	$\alpha = 3$	$\alpha = 1$	$\alpha = 2$	$\alpha = 3$
0	0.1305	2.4657	6.3604	-9.7862	0.0421	8.4659
1	-0.1428	0.5426	-1.0067	-0.0005	0.0151	-0.1798
2	0.0204	0.0784	0.0529	0.0000	0.0001	0.0091
3	-0.0048	0.0481	-0.1107	-0.0000	0.0000	-0.0008
4	0.0014	0.0225	0.0140	0.0000	0.0000	0.0001

TABLE I. The first five Fourier coefficients $\hat{\omega}_{n\alpha}$ of the lowest energy bands for two values of the amplitude potential.

In general, one can conclude that the greater $|A|$ is, the better the linear part obeys the nearest neighbour approximation, which is intuitively expected since the probability of tunelling between neighbor potential wells decreases with the amplitude of the potential. At the same time, if A is fixed the coefficients $\hat{\omega}_{n,\alpha}$, $n = 0, \pm 1, ..$ decay faster for lower bands α. The results illustrate, that the nearest neighbor approximation works for both potential amplitudes, while the averaging resulting in (12) is applicable for $A = -15$ but not for $A = -1$. The reason is that in the latter case the frequencies of oscillating exponents in (iii) are of order of $\omega_{1,\alpha}$.

Moving to assumption (ii), let us introduce the following notation. We denote by $N_{\alpha,m}^n(\Delta)$ the number of coefficients $W_{\alpha\alpha_1\alpha_2\alpha_3}^{0n_1n_2n_3}$, $|n_i| \leq n$, $\alpha_j \leq m$, $i, j = 1, 2, 3$ (the coefficients with permuted indices are regarded as different) such that $|W_{\alpha\alpha_1\alpha_2\alpha_3}^{0n_1n_2n_3}| > \Delta$. As it is clear Δ plays the role of the small parameter of the second condition, and $N_{\alpha,m}^n(\Delta)$ gives the number of sites/zones necessary to take into account for maintaining the given accuracy. In the cases of the amplitudes $A = -1$ and $A = -15$ we have obtained that $N_{1,1}^n(0.1) = N_{1,1}^n(0.01) = 1$ for $n = 1, ..., 5$. For $N_{1,m}^n(0.1)$ and $N_{1,m}^n(0.01)$, see Table II.

A	n	$N_{1,2}^n(0.1)$	$N_{1,2}^n(0.01)$	$N_{1,3}^n(0.1)$	$N_{1,3}^n(0.01)$
-1	0	4	4	7	13
	1	4	48	7	219
	2	4	54	7	249
	3, 4	4	60	7	303
	5	4	60	7	339
-15	0	4	4	13	14
	$1 - 5$	4	4	13	26

TABLE II. The values $N_{\alpha,m}^n(\Delta)$.

Table III presents the overlapping coefficients $W_{\alpha\alpha_1}$ for two values of the amplitude of the cos-like potential.

A	W_{11}	W_{22}	W_{33}	W_{12}	W_{13}	W_{23}
-1	0.375	0.240	0.173	0.182	0.152	0.142
-15	0.892	0.623	0.473	0.417	0.262	0.326

TABLE III. Overlapping coefficients $W_{\alpha\alpha_1}$.

It follows from Tables II and III that, in general *one cannot neglect the contribution of the WF of the highest zones.* However, one can show that the model (11) can be successfully used to describe bright monochromatic GS solutions of (1) of the form $\psi(t,x) = e^{i\omega t}u(x)$. An example is shown in Fig. 1 for (the "intermediate" between the above presented ones case of) $A = -5$. The two panels show the cases of $\omega = -1.5$ (left panels) and $\omega = 1.5$ (right panels), for $\sigma = 1$. The top panels show the comparison of the exact solution (shown by solid line) of Eq. (1) with the reconstructed profile obtained from solving Eq. (12) and using Eq. (7). The relevant profiles in the tight binding approximation are shown by dashed line, while in the right panel (where the one band approximation is less accurate), the 3-band approximation is also shown by dash-dotted line. The bottom panels show in a semilog plot the square modulus of the configurations of the top panels as well as, additionally, by dotted line the result of time evolution (for $t \approx 50$) of Eq. (1) with the tight binding approximation as the initial condition of the simulation. One can straightforwardly observe that the approximate solution "reshapes" itself into the exact solution (possibly shedding some very small amplitude radiation wakes in the process). This demonstrates that

the method can be used very efficiently to construct (approximate) solutions of the original PDE, by using the lattice reduction in the WF representation.
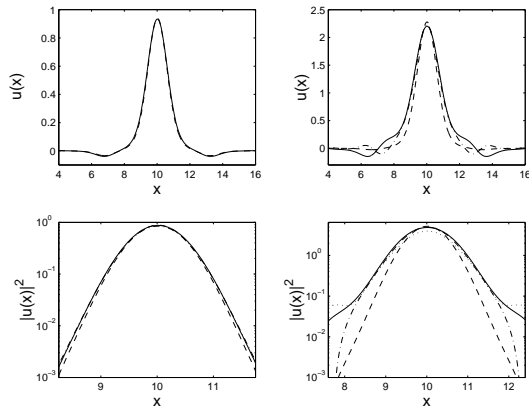

FIG. 1. Comparison of the lattice reconstructed solution in the tight binding (dashed line) and the 3-band (dash-dotted line) approximation with the exact solution (solid line). The comparison is performed for $A = -5$ and $\omega = -1.5$ (left panels) and $A = -5$, $\omega = 1.5$ (right panels). In the bottom (semilog) panels additionally the result of dynamical time evolution of the tight binding approximation is shown by the dotted line. The latter can be seen to approach, as time evolves (the shown snapshots are for $t \approx 50$), the shape of the exact solution (in the left panel it can actually not be distinguished from it) and to match its asymptotics, possibly shedding small wakes of low amplitude wave radiation in the process (see e.g., the bottom right panel).

Let us return now to the requirement (iii) and argue that choosing the small parameter as $\epsilon = |A|^{-1}$ one can provide averaging of (1) in the limit $A \to -\infty$. Namely, we claim that

(a) If α is fixed and $A \to -\infty$ then

$$\hat{\omega}_{0,\alpha} \sim A + (2\alpha - 1)\sqrt{-A} + ((2\alpha - 1)^2 + 1)/8\,.$$

If A is fixed then $\hat{\omega}_{0,\alpha}$ tends to infinity as α grows;

(b) If α is fixed then the value $\hat{\omega}_{1,\alpha}$ tends to zero faster than any power of $1/|A|$; at the same time if A is fixed then $\hat{\omega}_{1,\alpha}$ tends to infinity as α grows;

(c) If α is fixed and $A \to -\infty$ the Wannier functions can be approximated by the formula

$$w_{0,\alpha}(x) \approx \frac{(2|A|)^{\frac{1}{8}}}{\pi^{\frac{1}{4}}\sqrt{2^{\alpha-1}(\alpha-1)!}} e^{-\sqrt{\frac{|A|}{2}}x^2} H_{\alpha-1}\left((2|A|)^{\frac{1}{4}}x\right)$$

where $H_k(y)$ are Hermite polynomials. This is a natural consequence of the fact that for sufficently low levels the potential can be well approximated by the parabolic one;

(d) The coefficients $W^{nn_1n_2n_3}_{\alpha\alpha_1\alpha_2\alpha_3}$ with different n,n_1,n_2 and n_3 tend to zero as $A \to -\infty$ and at the same time $W^{nnnn}_{\alpha\alpha_1\alpha_2\alpha_3} \approx K_{\alpha\alpha_1\alpha_2\alpha_3}|A|^{\frac{1}{4}}$ where $K_{\alpha,\alpha_1,\alpha_2,\alpha_3}$ do not depend on A and can be expressed explicitly through the integrals of products of Hermite polinomials [12].

Taking into account (a)-(d), making the substitution $c_{n,\alpha}(t) = e^{i\omega_{0,\alpha}t}|A|^{-1/8}\tilde{c}_{n,\alpha}(t)$ and averaging over rapid oscillations one arrives at (12) with $W_{\alpha\alpha_1} = K_{\alpha\alpha_1\alpha\alpha_1}$.

To conclude we have shown how to derive lattice models which approximate efficiently nonlinear partial differential equations with periodic coefficients. This analysis gives the possibility to control the validity of the tight-binding approximation. In particular, we have shown that in a large region of parameter space, for the cos-like potential, one cannot restrict consideration to the lowest band. This is due to interband transitions originating from the nonlinearity (a situation very different from the one known in the (linear) solid-state physics, where the interband transitions occur due to effect of perturbations). However, there exist parameter ranges where with reasonably high accuracy the atomic wave function (that is a bright gap soliton of the 1D NLS equation) is approximated by a single WF. Such a state will form a "Wannier-soliton" that should also be experimentally observable. It should be highlighted that the use of the WF basis allows one to test, extend and improve the tight-binding approximation, in a *controllable* and *systematic* fashion by accounting for higher order terms in the Wannier expansion. Moreover, there is a computational gain when computing with a discrete system with respect to the corresponding cost for a much finer mesh (needed to resolve the original continuous system). While this gain may not be overly significant in one dimension, it may prove quite useful in tackling higher dimensional problems.

It should be stressed that even though developed for a specific, physically relevant (to optical lattices in BEC) setting, the approach presented here is *very general* and *directly applicable* to numerous other physical problems including the description of solitary wave propagation through one-dimensional photonic crystals, [16] chemical reactions on periodic catalytic substrates, [17] or even population dynamics in appropriately heterogeneous substrates. [18].

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