Wannier functions analysis of the nonlinear Schrödinger equation with a periodic potential

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In the present paper 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 the Bose-Einstein condensate theory as well as to other physical systems, such as, 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., Ref. [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's) (also called *breathers*) [6,7], in a rather simple way. These entities correspond to *gap solitons* of the original continuum model [8]. 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 context it should also be mentioned that the reduction of a nonlinear evolution equation with periodic coefficients to a lattice model, and thus to the study of the corresponding map, is known to be possible in the case of a special potential of the form of a sum of Dirac-delta functions [9].

In this work we propose to use Wannier functions (WF) [4,10] 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 have recently been used both in connection with BEC in optical lattices [11] and with gap solitons in nonlinear photonic crystals [12]. 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 analyze the applicability of the tight-binding model. In particular, we argue that although the ILM's reported in Ref. [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 (NLS) equation

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

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where $\sigma=\pm 1$ and $V(x)$ is a periodic potential $V(x+L)=V(x)$ [16]. Consider the eigenvalue problem associated with Eq. (1),

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

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 that labels energy bands $E_\alpha(k)$. As is well known [4,10] $E_\alpha(k+[2\pi/L])=E_\alpha(k)$; thus one can represent the energy as a Fourier series,

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

where an asterisk stands for complex conjugation and

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

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

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

Conversely,

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

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 Eq. (5), can be made real and exponentially decaying at infinity [10]. 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 Eq. (1) can be expressed in the form

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

which after substitution in Eq. (1) gives

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

where

$$W^{nn_1n_2n_3}_{\alpha\alpha_1\alpha_2\alpha_3}=\int_{-\infty}^{\infty} w_{n,\alpha}w_{n_1,\alpha_1}w_{n_2,\alpha_2}w_{n_3,\alpha_3}dx \tag{9}$$

are overlapping matrix elements. Since WF's are real, $W^{n_1n_2n_3n_4}_{\alpha_1\alpha_2\alpha_3\alpha_4}$ 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). Equation (8) can be viewed as a vector discrete nonlinear Schrödinger (DNLS) equation for $\mathbf{c}_n=\mathrm{col}(c_{n1},c_{n2},\dots)$ 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 $W^{nn_1n_2n_3}_{\alpha\alpha_1\alpha_2\alpha_3}$ those with $n=n_1=n_2=n_3$ are dominant and other terms can be neglected.

Then, taking into account this and point (i) one arrives at the equation

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

which degenerates into the tight-binding model [6]

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

if one restricts consideration to 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 intersite nonlinearities of the same type as in the model introduced in Ref. [13]. It should also be mentioned that the coefficients $W^{nnnn}_{\alpha\alpha_1\alpha_2\alpha_3}$ 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 time scale $1/\epsilon$ these exponents are rapidly oscillating

unless $\alpha=\alpha_2,\alpha_1=\alpha_3$ or $\alpha=\alpha_3,\alpha_1=\alpha_2$. Then, denoting $W^{nnnn}_{\alpha\alpha_1\alpha\alpha_1}\equiv W_{\alpha\alpha_1}$ (the coefficients $W_{\alpha\alpha_1}$ do not depend on n and describe interband interactions), and using time averaging techniques [15], one can reduce the lattice equation (10) to the form

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

This is a vector DNLS equation with coupling between bands of the cross phase modulation type [16,17]. 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. First, 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. Second, 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 $W^{nn_1n_2n_3}_{\alpha\alpha_1\alpha_2\alpha_3}/W^{nnnn}_{\alpha\alpha_1\alpha_2\alpha_3}$ $(n_j\neq n)$ 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 paper 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. The lowest band gaps of its spectrum are shown in Fig. 1 for three values of the potential amplitude: $A=-1$, $A=-5$, and $A=-15$, taken as representative examples of low, moderate, and high potential barriers, respectively (although not reported here, intermediate values of A were also considered). We remark that for very large potential amplitudes, difficulties in numerical studies usually arise because of the very small width of the allowed bands [c.f. Figs. 1(a) and 1 (c)]. This case, however, allows a rather complete and satisfactory asymptotic analysis (see below).

Next, Table I shows the coefficients $\hat{\omega}_{n,\alpha}$ for the same three lowest energy bands. Our numerical investigations, realized for various values of A, show that the greater $|A|$ is, the better the linear part obeys the nearest neighbor approximation, which is intuitively expected since the probability of tunneling between neighbor potential wells decreases with the amplitude of the potential. At the same time, if A is fixed, the coefficients $\hat{\omega}_{n,\alpha}$, $n=0,\pm1,\ldots$ decay faster for lower bands α. The results illustrate, that the nearest neighbor approximation works for all three potential amplitudes, while the averaging resulting in (12) is applicable for $A=-15$ and even for $A=-5$, but not for $A=-1$. The reason is that in the latter case the frequencies of oscillating exponents in (iii) are of the order of $\omega_{1,\alpha}$.

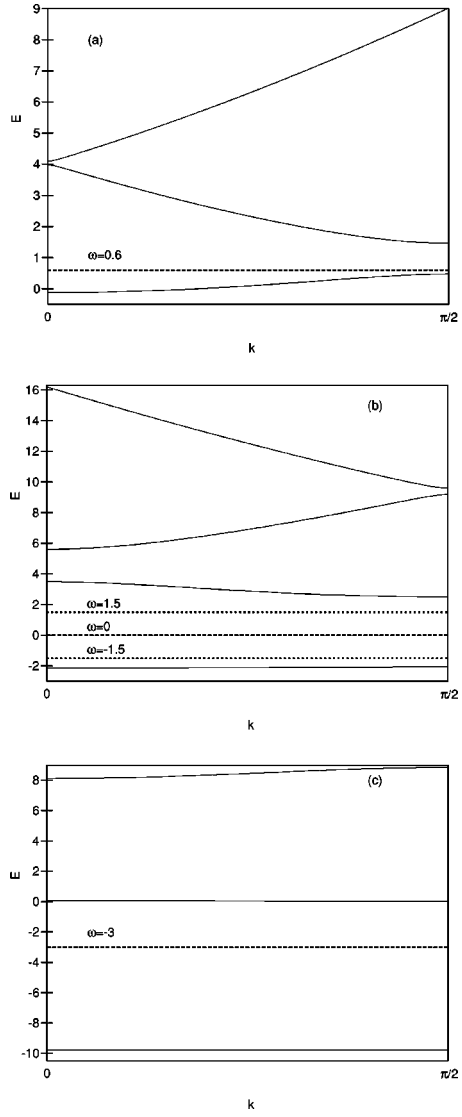

FIG. 1. The energy band structure (given by the solid lines) of the potential $V=A\cos(2x)$ for three different values of the amplitude (a) $A=-1$, (b) $A=-5$, and (c) $A=-15$ (in the last case the first three allowed bands appear to be very narrow: $[-9.787, -9785]$, $[0.012,0.073]$, and $[8.123,8.846]$). Dashed lines in each picture show positions of the frequencies of the localized solutions analyzed in Table IV and those represented in Fig. 2.

Moving to assumption (ii), let us introduce the following notation. We denote by $N^n_{\alpha,m}(\Delta)$, the number of coefficients $W^{0n_1n_2n_3}_{\alpha\alpha_1\alpha_2\alpha_3}$, $|n_i|\leqslant n$, $\alpha_j\leqslant m$, $i,j=1,2,3$ (the coefficients with permuted indices are regarded as different) such that $|W^{0n_1n_2n_3}_{\alpha\alpha_1\alpha_2\alpha_3}|>\Delta$. As it is clear, Δ plays the role of the small parameter of the second condition, and $N^n_{\alpha,m}(\Delta)$ 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 $N^n_{1,1}(0.1)=N^n_{1,1}(0.01)=1$ for $n=1,\ldots,5$. For $N^n_{1,m}(0.1)$ and $N^n_{1,m}(0.01)$, see Table II.

Table III presents the overlapping coefficients $W_{\alpha\alpha_1}$ for three values of the amplitude of the cosinelike potential.

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

	$A=-1$			$A=-5$			$A=-15$		
n	$\alpha=1$	$\alpha=2$	$\alpha=3$	$\alpha=1$	$\alpha=2$	$\alpha=3$	$\alpha=1$	$\alpha=2$	$\alpha=3$
0	0.1305	2.4657	6.3604	−2.1152	2.9389	7.0721	−9.7862	0.0421	8.4659
1	−0.1428	0.5426	−1.0067	−0.0192	0.2435	0.7939	−0.0005	0.0151	−0.1798
2	0.0204	0.0784	0.0529	0.0002	0.0263	0.1094	0.0000	0.0001	0.0091
3	−0.0048	0.0481	−0.1107	−0.0000	0.0052	0.0625	−0.0000	0.0000	−0.0008
4	0.0014	0.0225	0.0140	0.0000	0.0012	0.0290	0.0000	0.0000	0.0001

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 ground state solutions of (1) of the form $\psi(t,x)=e^{i\omega t}u(x)$. To this end, we present in Table IV the first coefficients of the expansion of the exact (numerical) solution of Eq. (1) for the cases of potential amplitudes considered above, and for typical values of soliton frequencies inside the forbidden bands.

It follows from the data shown in Table IV that the tight-binding model is not applicable for the case of small amplitudes of the potential: for $A=-1$ one has to take into account at least five WF's corresponding to the first Brillouin zone (from $c_{0,1}$ till $c_{3,1}$), while contribution of higher zones, described by $c_{n,\alpha}$ with different index α, can be neglected. Notice that by increasing the potential amplitude, there is a more significant contribution of the upper zones and a relatively accurate description of the soliton in terms of the WF's. Indeed, already for $A=-5$ (and the same for $A=-15$), the leading order coefficient $c_{0,1}$ is ten times bigger than any other coefficient of the expansion, the next one (with respect to the magnitude) being $c_{0,3}$, i.e., the coefficient of the WF belonging to the same site, but to the third zone. In this case the solution can be identified as a *Wannier soliton*, i.e., a solitary wave solution which is described, with high accuracy, by a single WF.

In Fig. 2 we provide comparison among exact, lattice, and tight-binding solutions for the 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 a dashed line, while in the right panel (where the one-band approximation is less accurate), the three-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 the 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 partial differential equation, by using the lattice reduction in the WF representation.

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

A	n	$N^n_{1,2}(0.1)$	$N^n_{1,2}(0.01)$	$N^n_{1,3}(0.1)$	$N^n_{1,3}(0.01)$
−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
−5	0	4	4	10	14
	1	4	10	10	62
	2	4	10	10	74
	3−5	4	10	10	86
−15	0	4	4	13	14
	1−5	4	4	13	26

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

(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

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

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

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
−5	0.648	0.398	0.279	0.270	0.162	0.210
−15	0.892	0.623	0.473	0.417	0.262	0.326

TABLE IV. The expansion coefficients $c_{n,\alpha}$ of exact (numerical) solutions of the NLS (1) with the potential $V=A\cos(2x)$.

	α	$n=0$	$n=1$	$n=2$	$n=3$	$n=4$	$n=5$	$n=6$
$A=-1$	1	0.809	−0.526	0.289	−0.158	0.088	−0.049	0.027
$\omega=0.6$	2	0.000	0.023	−0.014	0.009	−0.003	0.002	0.000
	3	−0.013	0.000	0.000	−0.001	0.000	0.000	0.000
$A=-5$	1	1.895	−0.023	−0.001	0.000	0.000	0.000	0.000
$\omega=0$	2	0.000	0.056	0.004	0.001	0.000	0.000	0.000
	3	−0.149	−0.023	−0.003	0.000	0.001	0.001	−0.001
$A=-15$	1	2.948	0.000	0.001	0.000	0.000	0.000	0.000
$\omega=-3$	2	0.000	0.008	0.001	0.000	0.000	0.000	0.000
	3	−0.385	0.002	−0.001	0.000	0.000	0.000	0.000

where $H_k(y)$ are Hermite polynomials. This is a natural consequence of the fact that for sufficiently 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 $W^{nnnn}_{\alpha\alpha_1\alpha_2\alpha_3}\approx K_{\alpha\alpha_1\alpha_2\alpha_3}|A|^{1/4}$, 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 polynomials [14].

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 Eq. (12) with $W_{\alpha\alpha_1}=K_{\alpha\alpha_1\alpha\alpha_1}$.

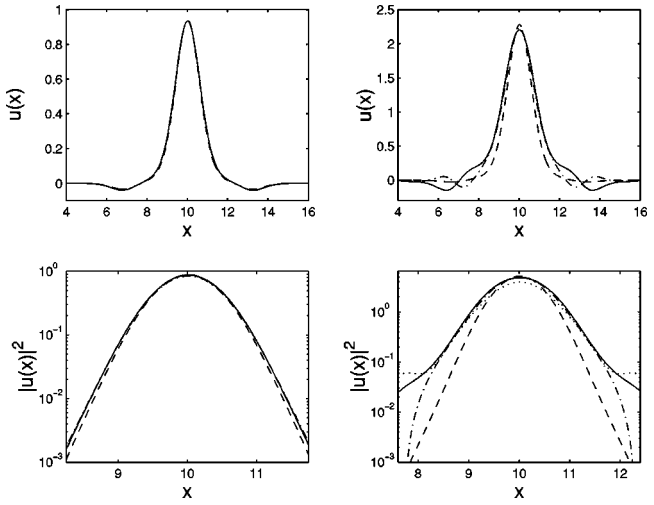

FIG. 2. Comparison of the lattice reconstructed solution in the tight-binding (dashed line) and the three-band (dash-dotted line) approximation with the exact solution (solid line). The comparison is performed for $A=-5$ and $\omega=-1.5$ (left panels) and $A=-5$, $\omega=1.5$ (right panels). The positions of both frequencies with respect to gap edges are shown in Fig. 1(b). 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).

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 cosinelike potential, one cannot restrict consideration to the lowest band. This is due to interband transitions originating from the nonlinearity [a situation very different from that known in (linear) solid-state physics, where the interband transitions occur due to the 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 one-dimensional 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 [18], chemical reactions on periodic catalytic substrates [19], or even population dynamics on appropriately heterogeneous substrates [20].

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