New approximation for nonlinear evolution in periodic potentials

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A new approximation for evolution described by Nonlinear Schrödinger Equation (NLS) with periodic potential is presented. It relies on restricting dynamics to one band of the bandgap spectrum, and taking into account only one, dominating Fourier component in the nonlinear Bloch-wave mixing. The resulting equation has a simple, discrete form in the basis of linear Wannier functions, and turns out to be very accurate as long as the modes in other bands are not excited and the potential is not very deep. Widely used approximations, the tight-binding approximation and the effective mass approximation, are derived from the new equation as the limiting cases.

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The Nonlinear Schrödinger Equation (NLS) is one of the most common and basic nonlinear wave equations. Recent experimental progress in the fields of nonlinear optics and Bose-Einstein condensation, where it is known as the Gross-Pitaevskii equation, has strongly stimulated theoretical studies on its properties and solutions. The ability to describe and understand nonlinear evolution in periodic potentials is of a great practical importance, since this kind of potential can be easily created by a periodically varying refractive index of an optical medium [1, 2, 3, 4], or by a standing laser wave imposed on a Bose-Einstein condensate [5, 6]. On the other hand, the presence of a periodic potential can dramatically modify the wave diffraction, and creates a way to control the nonlinear evolution of physical systems.

To date, there are a few models commonly used to describe these systems in a simplified way. In the case of a deep potential, the essential properties of system dynamics are included in the tight-binding (or coupled-mode) approximation, which assumes that the interaction of neighbouring cells can be described by tunneling between their localized modes. As a result of this assumption, one obtains a Discrete Nonlinear Schrödinger Equation (DNLS), a very convenient tool for studying the pseudomomentum will be denoted with \( k' \). For each \( k' \in (-\pi, \pi) \), there exists a Bloch function \( \nu(x, k') \) of energy \( E(k') \), and its Fourier transform \( \nu(k, k') \) is the solution of the linear version of Eq. (2)

\[
E(k')\nu(k, k') = k'^2\nu(k, k') + \sum_n U_n\nu(k - 2\pi n, k'),
\]

with orthonormality condition \( \int \nu(k, k'_1)\nu^*(k, k'_2)dk = \delta(k'_1 - k'_2) \). It is assumed that the solution is the superposition of Bloch functions of the chosen band

\[
\tilde{u}(k, t) = \int_{-\pi}^{\pi} \tilde{\phi}(k', t)\nu(k, k')dk'.
\]

This assumption implies that the nonlinearity is rather weak, since strong nonlinearity leads to Bloch wave mixing of waves in different bands, or even destruction of

\[
\frac{\partial u}{\partial t} + k^2u + U(x)u + \sigma|u|^2u = 0,
\]

where \( U(x) + 1 = U(x) \in \mathbb{R} \) and \( \sigma = \pm 1 \) is the sign of the nonlinearity. The norm of the solution \( N = \int_{-\infty}^{+\infty} |u|^2dx \) is a constant of motion. After performing Fourier transform one obtains the equation for \( \hat{u}(k, t) = (2\pi)^{-1/2} \int_{-\infty}^{+\infty} u(x, t)e^{-ikx}dx \)

\[
\frac{\partial \hat{u}(k)}{\partial t} = -k^2\hat{u}(k) - \sum_n U_n\hat{u}(k - 2\pi n) + \frac{\sigma}{2\pi} \int_{-\infty}^{+\infty} u(k_1)u^*(k_2)u(k - k_1 + k_2)dk_1dk_2,
\]

where \( U(x) = \sum_n U_n\delta(2\pi nx) \), and the integer index \( n \in (-\infty, +\infty) \). From now on the dynamics will be restricted to one certain band of the bandgap spectrum.
the band structure \[5\]. After substituting this equation respectively. c), d) Same as a), b), but for potential depth \(\varepsilon = 10\).

FIG. 1: (color online) a) Linear Bloch wave spectrum in cosine potential of depth \(\varepsilon = 4\). Small dots correspond to frames in Fig. 2 b) Contribution of the main component in decomposition of a Bloch wave in Fourier space. Dashed and solid lines correspond to the first and the second band, respectively. c), d) Same as a), b), but for potential depth \(\varepsilon = 10\).

As a result, the above equation takes the form
\[
i \frac{\partial \tilde{\phi}(k', t)}{\partial t} = - E(k') \tilde{\phi}(k', t) + \frac{\sigma}{2\pi} \int_{-\pi}^{\pi} \tilde{\phi}(k', t) \tilde{\phi}^*(k''_1, t) \tilde{\phi}(k''_2, t) dk''_1 dk''_2 dk' dtk'.
\]

Inverse Fourier transform gives a simple discrete equation, which is the main result of this letter
\[
i \frac{d\phi_n}{dt} = - \sum_m E_m \phi_{n-m} + \sigma |\phi_n|^2 \phi_n. \tag{5}
\]

Here \(\tilde{\phi}(k', t) = (2\pi)^{-1/2} \sum_n \phi_n(t) e^{-ik't} \) and \(E(k') = \sum_n E_n e^{-ik'n} \). The norm of the discrete function is \(\sum_n |\phi_n|^2 = N\). Most of the terms in the infinite sum can be neglected, since absolute values of \(E_m\) are significant only for \(m\) close to zero. In numerical simulations presented below, only terms with \(|m| \leq 5\) were taken into account. Values of \(E_m\) can be found quite easily, by solving a linear eigenvalue problem \[3\] (see e.g. \[5\]) and performing an inverse Fourier transform.

The scheme of the above derivation is similar to the one presented in \[8\], where a vector discrete equation was obtained for evolution in the basis of Wannier functions. In fact, the one-band assumption imply that the function \(u(x, t)\) can be approximated by
\[
u(x, t) = \sum_n \phi_n(t) w(x - n), \tag{6}
\]

where \(w(x) = w(x) = \int_{-\infty}^{\infty} u(x, t) dk'\). Therefore, \(\phi_n\) can be interpreted as the amplitude of the wavefunction in the \(n\)-th site of the periodic potential.

It is relevant to point out possible generalizations of the presented model. The one-band approximation can be extended to include more than one band. In this case, one would obtain a system of discrete equations \[8\], each of them coupled with others by cross-phase modulation terms. The deviation can also be easily generalized to the case of multi-dimensional NLS equation \[11\]. However, one has to be aware that in this case the nonlinear mixing between bands is more likely to occur, since the band gaps are not always closed \[11\]. Finally, the presented method can be applied to other types of nonlinearity, e. g. quadratic, cubic-quintic, or other nonlinearities after expanding them in Taylor series. A detailed study on these generalizations will be presented elsewhere.

Equation \[5\] has two interesting limiting cases. For a deep potential, the energy dependence \(E(k')\) becomes close to the cosine function, and the infinite sum can be approximated by three terms with \(m = -1, 0, 1\). This form of the equation is equivalent to the one obtained...
and expanding $\Phi(x, t)$ order leads to the effective mass equation

$$i \frac{\partial \Phi}{\partial t} = -E(k_0^\prime)\Phi - iv_s \frac{\partial \Phi}{\partial x} + \frac{1}{m_{\text{eff}}} \frac{\partial^2 \Phi}{\partial x^2} + \sigma |\Phi|^2 \Phi,$$

where $v_s = (dE/dk')|_{k' = k_0^\prime}$ is the group velocity, and $m_{\text{eff}} = (d^2E/dk'^2)^{-1}|_{k' = k_0^\prime}$ is the effective mass. In this case, the new equation works quantitatively with the NLS equation. This is confirmed by numerical simulations, see Fig. 2.

To test the new approximation, the equation was applied to description of band-gap solitons. These states are the inherently nonlinear solutions of the NLS equation in the form $u(x, t) = u(x) \exp(-i\beta t)$, where $\beta$ is the eigenvalue of the soliton, lying in the gap of the band-gap spectrum. In Fig. 2 these states are compared with analogous solutions of Eq. 5, $\phi_n(t) = \phi_n \exp(-i\beta t)$ and the corresponding functions $u, \phi$, cf. Eq. 4. In particular, the two figures a), b) present solutions of the same equation, describing evolution in the lowest band, with the only change in the sign of the nonlinearity. The agreement with the full NLS solution is perfect. Interestingly, the solution in Fig. 2a) has larger width and norm than the solution in Fig. 2b).

In the tight-binding model, solitons with larger norm always has a smaller width, independently on the sign of nonlinearity. Here, the new equation takes into account the difference in diffraction strength at the top and the bottom of the first band. In Fig. 2b) a soliton composed of Bloch waves from the second band is shown. In this case, maxima of amplitude lie on maxima of the periodic potential. The agreement between the full model and the approximate model is in this case somewhat inferior. Additional simulations have shown that the reason for this is the strength of the nonlinearity; the eigenvalue of the solution is shifted deeper into the band gap than in the previous cases. In general, the equation works best if the nonlinear energy is much smaller than both the gap width and the band width.

In Fig. 2 a systematic comparison of the full and approximate models is presented. Here the width and maximum amplitude of the lowest-energy soliton is depicted versus the potential depth $\varepsilon$. Good agreement of calculated width $W(u) = 3 \int |x||u(x)|^2 dx / \int |u(x)|^2 dx$ suggests that the shape of the approximate solution is correct even for very strong potentials, with the only difference in the norm $N$.

The new approximation can also describe dynamical evolution problems. A very simplified version of it was...
FIG. 4: (color online) Motion of a soliton wavepacket with imprinted linear phase for $N = 3$ and $\varepsilon = 4$, according to a) the NLS equation and b) the discrete equation (5). c), d) Same as in a), b), but for $\varepsilon = 10$. In this case, the soliton is trapped by the Peierls-Nabarro potential. The shape of solitons is the same as in Fig. 2b).

already used for justification of the phenomenon of spontaneous migration of Bloch waves to the regions of normal diffraction for positive nonlinearity, and to the regions of anomalous diffraction for negative one [7]. This nonlinear phenomenon was observed experimentally in two different systems [13], and can be utilized for efficient soliton generation [7]. Here the new model is used to describe soliton mobility, see Fig. 4. The lowest-energy soliton wavepacket was “boosted” by imprinting a linear phase $u(x, 0) = u(x) \exp(ikx)$, with $k = 0.1$. In the case of a weak potential, the wavepacket started to move with a constant velocity. In the case of a deep potential, it has been trapped in central sites by the Peierls-Nabarro potential [14]. This effect would not be seen within the usual effective mass approximation. Here, the agreement between the NLS equation and Eq. (5) is very good for the weak potential, worse for the deep potential, but the main effect is still apparent.

In conclusion, a new approximation for evolution described by Nonlinear Schrödinger Equation with periodic potential was presented. The derivation is based on the one-band approximation and simplification of nonlinear Bloch-wave mixing, and leads to a simple discrete equation in the basis of linear Wannier functions. The equation works very good as long as the nonlinearity does not cause excitation of modes in other bands and the potential is not very deep. The new model was used for description of gap solitons and a dynamical evolution. It was shown that the tight-binding approximation and the effective mass approximation can be derived from the new equation as the limiting cases. Possible generalizations were pointed out.

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