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Bifurcation of gap solitons in periodic potentials with a periodic sign-varying nonlinearity coefficient

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We address the Gross–Pitaevskii equation with a periodic linear potential and a periodic sign-varying nonlinearity coefficient. Contrary to the claims in the previous works, we show that the intersite cubic nonlinear terms in the discrete nonlinear Schrödinger (DNLS) equation appear beyond the applicability of assumptions of the tight-binding approximation. Instead of these terms, for an even linear potential and an odd nonlinearity coefficient, the DNLS equation and other reduced equations have the quintic nonlinear term, which correctly describes bifurcation of gap solitons in the semi-infinite gap.

Keywords: Gross–Pitaevskii equation; discrete nonlinear Schrödinger equation; gap solitons; bifurcations; semi-classical limit; Wannier functions

AMS Subject Classifications: 35Q55; 37K60

1. Introduction

The generalized discrete nonlinear Schrödinger (DNLS) equation with intersite cubic nonlinear terms,

$$\begin{aligned} i\dot{c}_n &= \alpha(c_{n+1}+c_{n-1})+\beta|c_n|^2c_n \\ &\quad +\gamma(2|c_n|^2(c_{n+1}+c_{n-1})+c_n^2(\bar{c}_{n+1}+\bar{c}_{n-1})+|c_{n+1}|^2c_{n+1}+|c_{n-1}|^2c_{n-1}) \\ &\quad +\delta((c_{n+1}^2+c_{n-1}^2)\bar{c}_n+2(|c_{n+1}|^2+|c_{n-1}|^2)c_n), \end{aligned} \tag{1.1}$$

where $(\alpha,\beta,\gamma,\delta)$ are constant parameters and the dot denotes differentiation in time, was derived independently in various contents. Smerzi and Trombettoni [1] suggested that this equation models Bose–Einstein condensates in a lattice, when Wannier functions associated with a periodic potential are replaced by the nonlinear bound states. Independently, this equation was derived heuristically by Oster et al. [2] to model waveguide arrays in a nonlinear photonic crystal. Earlier, the same equation

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was obtained by Claude et al. [3] for the modelling of slowly varying discrete breathers in the Fermi–Pasta–Ulam lattices using asymptotic multi-scale expansions. Very recently, the generalized DNLS equation was rederived again by Abdullaev et al. [4] in a more specific context of the Gross–Pitaevskii (GP) equation with a periodic potential and a periodic sign-varying nonlinearity coefficient. If the coefficient in front of the onsite cubic nonlinear term of the DNLS equation vanishes because of the sign-varying nonlinearity of the GP equation (i.e. if $\beta = 0$ in (1.1)); the authors of [4] incorporated other intersite cubic nonlinear terms from a decomposition involving Wannier functions.

In what follows, we focus on the specific application of the generalized DNLS equation (1.1) in the context of Bose–Einstein condensates in a lattice. Therefore, we consider the GP equation with a periodic linear potential and a periodic sign-varying nonlinearity coefficient in the form

$$i\partial_t \Psi = -\partial_x^2 \Psi + V(x)\Psi + G(x)|\Psi|^2\Psi, \tag{1.2}$$

where $V(x)$ and $G(x)$ are smooth, 2π-periodic functions on $\mathbb{R}$. To make all arguments precise, we assume that

$$V(-x) = V(x), \quad G(-x) = -G(x), \quad x \in \mathbb{R}, \tag{1.3}$$

which ensures that $\beta = 0$. In this case, our main result states that the intersite cubic nonlinear terms in the generalized DNLS equation (1.1) appear beyond the applicability of the DNLS equation in the tight-binding approximation and hence must be dropped from the leading order of the asymptotic equation. Instead of these terms, the onsite quintic nonlinear term must be taken into account to balance the linear dispersion term in the quintic DNLS equation

$$i\dot{c}_n = \alpha(c_{n+1} + c_{n-1}) + \chi|c_n|^4 c_n, \tag{1.4}$$

where (α, χ) are constant parameters which are computed from the semi-classical analysis of the GP equation (1.2) with potentials (1.3) (Theorem 2).

Note that the approach leading to the DNLS equation is general and can be applied to other 2π-periodic functions $V(x)$ and $G(x)$. In a general case, $\beta \neq 0$ and the onsite cubic nonlinear term is the only nonlinear term, which must be accounted in the cubic DNLS equation

$$i\dot{c}_n = \alpha(c_{n+1} + c_{n-1}) + \beta|c_n|^2 c_n \tag{1.5}$$

at the leading order of the asymptotic expansion (Theorem 1).

To compare the outcomes of the generalized DNLS equation (1.1) with those of the quintic DNLS equation (1.4), we study bifurcations of gap solitons in the semi-infinite band gap. We show analytically that α and χ has equal *negative* signs in the semi-infinite band gap so that the quintic DNLS equation (1.4) always has a positive localized mode. This fact indicates that a bifurcation of a gap soliton in the semi-infinite gap always occurs in the GP equation (1.2) with potentials (1.3) (Theorem 3). Recall that this bifurcation does not occur if the nonlinearity coefficient is sign-definite and positive [5].

In contrary to the predictions of the quintic DNLS equation (1.4), we also show that the corresponding version of the generalized DNLS equation (1.1) does not admit localized solutions for any values of α and γ (when $\beta = \delta = 0$) at least in the slowly varying approximation. A numerical test with particular potentials

$$V(x) = V_0(1 - \cos(x)), \quad G(x) = G_0 \sin(x), \tag{1.6}$$

indicates that the gap solitons do exist in the semi-infinite gap independently of the signs of V_0 and G_0. The rigorous proof of the existence of localized solutions in the GP equation (1.2) with potentials (1.3) in the semi-infinite band gap is beyond the scopes of this work and is a subject of an ongoing work [6].

We also inspect another asymptotic reduction of the GP equation (1.2) to the continuous nonlinear Schrödinger (CNLS) equation (see review of asymptotic reductions of the GP equation with a periodic potential in [7]). We show that the corresponding CNLS equation also has a focusing quintic nonlinear term, which supports the same conclusion on bifurcation of a gap soliton in the semi-infinite gap.

We note that reductions to the DNLS and CNLS equations were recently justified with rigorous analysis both in the stationary and time-dependent cases (see [8,9] in the context of the DNLS equation and [10,11] in the context of the CNLS equation). Therefore, it is a matter of a routine technique to formalize arguments of our article.

We shall add that the physics literature on the GP equation with sign-varying nonlinearity coefficient is rapidly growing. The GP equation (1.2) with $V(x) \equiv 0$ and a nonzero mean value of $G(x)$ was considered by Fibich et al. [12]. For the same equation with zero mean value of $G(x)$, Sakaguchi and Malomed [13] derived a quintic CNLS equation in a slowly varying approximation of a broad soliton.

A more general equation with both linear and nonlinear periodic coefficients was studied by Bludov et al. in [14,15], where gap solitons were approximated numerically. It was shown in these works that bifurcations of small-amplitude gap solitons near the lowest band edge depend on the sign of the cubic coefficient in the effective CNLS equation. Using perturbation theory, Rapti et al. [16] studied the existence and stability of gap solitons in the semi-infinite gap for the GP equation with small linear and nonlinear periodic coefficients.

This article is organized as follows. Section 2 justifies the asymptotic reductions of the GP equation (1.2) to the quintic DNLS equation (1.4) and the cubic DNLS equation (1.5). Section 3 gives results on the existence of stationary localized modes in the GP equation (1.2) with potentials (1.3). Section 4 discusses the relevance of previous works [1] and [4] on the generalized DNLS equation (1.1). Section 5 describes the asymptotic reduction of the GP equation (1.2) to the quintic CNLS equation. Appendices A and B report details of the semi-classical analysis needed for the proof of main results.

2. Reductions to the DNLS equation

To consider the tight-binding approximation and reductions to the DNLS equation, we assume that

$$V(x) = \epsilon^{-2} V_0(x), \tag{2.1}$$

where ϵ is a small parameter and V_0 is a smooth, 2π-periodic, and even function on $\mathbb{R}$. In what follows and without loss of generality, we set

$$V_0(0) = 0 \quad \text{and} \quad V_0''(0) = 2, \tag{2.2}$$

so that $V_0(x) = x^2 + \mathcal{O}(x^4)$ as $x \to 0$. For particular explicit computations, we consider the standard example

$$V_0(x) = 2(1 - \cos(x)) = 4\sin^2\left(\frac{x}{2}\right).$$

The limit $\epsilon \to 0$ is generally referred to as the semi-classical limit [17]. Appendix A delivers important computations of the semi-classical analysis.

2.1. *Reduction to the cubic DNLS equation*

We will show that an asymptotic reduction to the cubic DNLS equation (1.5) holds for $\beta \neq 0$, where

$$\beta = \epsilon^{1/2} \int_{\mathbb{R}} G(x) \hat{\psi}_0^4(x) \mathrm{d}x$$

and $\hat{\psi}_0$ is the Wannier function for the lowest energy band described in Appendix A. Computations (A.8) and (A.9) in Appendix A suggest the use of the scaling transformation

$$\Psi(x, t) = \epsilon^{1/4} \mu^{1/2} (\Psi_0 + \mu \Psi_1) e^{-i\hat{E}_0 t}, \tag{2.3}$$

with a new small parameter

$$\mu = \frac{1}{\pi^{1/2} \epsilon^{3/2}} e^{-\frac{2}{\epsilon}\int_0^\pi \sqrt{V_0(x)}\mathrm{d}x}. \tag{2.4}$$

Let $T = \mu t$ be slow time and decompose

$$\Psi_0 = \sum_{n \in \mathbb{Z}} c_n(T) \hat{\psi}_n(x),$$

for some coefficients $\{c_n\}_{n \in \mathbb{Z}}$ to be defined. The remainder term Ψ_1 satisfies

$$\begin{aligned} i\partial_t \Psi_1 = (L - \hat{E}_0)\Psi_1 + \sum_{n \in \mathbb{Z}} \left(-i\dot{c}_n + \mu^{-1} \sum_{m \in \mathbb{N}} \hat{E}_m (c_{n+m} + c_{n-m}) \right) \hat{\psi}_n \\ + \epsilon^{1/2} G(x) |\Psi_0 + \mu \Psi_1|^2 (\Psi_0 + \mu \Psi_1). \end{aligned}$$

Coefficients $\{c_n\}_{n \in \mathbb{Z}}$ are uniquely defined by the orthogonality condition

$$\langle \hat{\psi}_n, \Psi_1 \rangle = 0 \quad \text{for all } n \in \mathbb{Z},$$

which ensures that Ψ_1 is in the orthogonal complement of the subspace of $L^2(\mathbb{R})$ corresponding to the lowest spectral band of operator L. Orthogonal projections to $\{\hat{\psi}_n\}_{n \in \mathbb{Z}}$ truncated at the leading-order terms as $\mu \to 0$ take the form of the cubic DNLS equation

$$i\dot{c}_n = \alpha(c_{n+1} + c_{n-1}) + \beta |c_n|^2 c_n, \tag{2.5}$$

where

$$\alpha = \mu^{-1} \hat{E}_1, \quad \beta = \epsilon^{1/2} \int_{\mathbb{R}} G(x) \hat{\psi}_0^4(x) \mathrm{d}x, \tag{2.6}$$

according to the fact that other overlapping integrals in the linear and cubic terms are smaller. By the computations (A.8) and (A.9) in Appendix A, we have

$$\alpha \sim -4\sqrt{V_0(\pi)}\exp\left(\int_0^{\pi}\frac{1-S'(x)}{S(x)}\mathrm{d}x\right), \quad \beta \sim \frac{1}{(2\pi)^{1/2}}G(0), \tag{2.7}$$

so that $\beta \neq 0$ if $G(0) \neq 0$. Note that if $G(0)=0$, β may be nonzero and the asymptotic solution (2.3) leading to the same cubic DNLS equation (2.5) will need to have a different algebraic power of ϵ.

Rigorous justification of the cubic DNLS equation (2.5) on a finite time interval is proved by Pelinovsky and Schneider [9], where the main result is formulated in space $\mathcal{H}^1(\mathbb{R})$ defined by the norm $\|\Psi\|_{\mathcal{H}^1} := \sqrt{\langle (L+I)\Psi, \Psi\rangle}$, where $L = -\partial_x^2 + V(x)$.

THEOREM 1 *Assume that* $V(x)$ *is given by* (2.1), $G(0)\neq 0$, *and* μ *is given by* (2.4). *Let* $\{c_n(T)\}_{n\in\mathbb{Z}} \in C^1(\mathbb{R}, l^1(\mathbb{Z}))$ *be a global solution of the cubic DNLS equation* (2.5) *with initial data* $\{c_n(0)\}_{n\in\mathbb{Z}} \in l_p^2(\mathbb{Z})$ *for any* $p > \frac{1}{2}$. *Let* $\Psi_0 \in \mathcal{H}^1(\mathbb{R})$ *satisfy the bound*

$$\left\| \Psi_0 - \epsilon^{1/4}\mu^{1/2}\sum_{n\in\mathbb{Z}} c_n(0)\hat{\psi}_n \right\|_{\mathcal{H}^1} \leq C_0\epsilon^{1/4}\mu^{3/2}$$

for some $C_0 > 0$. *There exist* $\mu_0 > 0$, $T_0 > 0$ *and* $C > 0$ *such that for any* $\mu \in (0, \mu_0)$, *the GP equation* (1.2) *with initial data* $\Psi(0) = \Psi_0$ *has a solution* $\Psi(t) \in C([0, T_0/\mu], \mathcal{H}^1(\mathbb{R}))$ *satisfying the bound*

$$\forall t \in [0, T_0/\mu]: \quad \left\| \Psi(\cdot, t) - \epsilon^{1/4}\mu^{1/2}\left(\sum_{n\in\mathbb{Z}} c_n(\mu t)\hat{\psi}_n\right)e^{-i\hat{E}_0 t} \right\|_{\mathcal{H}^1} \leq C\epsilon^{1/4}\mu^{3/2}.$$

2.2. *Reduction to the quintic DNLS equation*

We now assume that $G(x)$ is odd on $\mathbb{R}$, then $\beta = 0$ and the DNLS equation (2.5) becomes a linear equation. A modified asymptotic solution is needed to incorporate the leading order of the asymptotic expansion. We will show that the modified scaling

$$\Psi(x,t) = \epsilon^{-1/4}\mu^{1/4}\big(\Psi_0 + \mu^{1/2}\Psi_1 + \mu\Psi_2\big)e^{-i\hat{E}_0 t} \tag{2.8}$$

will reduce the GP equation (1.2) to the quintic DNLS equation (1.4) with $\chi \neq 0$ if $G'(0) \neq 0$. Again, let $T = \mu t$ be the slow time and define Ψ_0 and Ψ_1 by

$$\Psi_0 = \sum_{n\in\mathbb{Z}} c_n(T)\hat{\psi}_n(x), \quad \Psi_1 = \sum_{n\in\mathbb{Z}} |c_n(T)|^2 c_n(T)\hat{\varphi}_n(x),$$

where $\hat{\varphi}_n(x) = \hat{\varphi}_0(x - 2\pi n)$, $n \in \mathbb{Z}$ is a solution of

$$(L - \hat{E}_0)\hat{\varphi}_0(x) = -\epsilon^{-1/2}G(x)\hat{\psi}_0^3(x), \quad x \in \mathbb{R}, \tag{2.9}$$

under the orthogonality condition

$$\int_{\mathbb{R}} G(x)\hat{\psi}_0^4(x)\mathrm{d}x = 0. \tag{2.10}$$

The remainder term Ψ_2 satisfies

$$i\partial_t \Psi_2 = (L - \hat{E}_0)\Psi_2 + \sum_{n\in\mathbb{Z}} \left(-i\dot{c}_n + \mu^{-1} \sum_{m\in\mathbb{N}} \hat{E}_m (c_{n+m} + c_{n-m}) \right) \hat{\psi}_n$$
$$- i\mu^{1/2} \sum_{n\in\mathbb{Z}} \frac{\mathrm{d}}{\mathrm{d}T} \left(|c_n|^2 c_n \right) \hat{\varphi}_n + \epsilon^{-1/2} \mu^{-1/2} G(x)$$
$$\times \left(|\Psi_0 + \mu^{1/2}\Psi_1 + \mu\Psi_2|^2 (\Psi_0 + \mu^{1/2}\Psi_1 + \mu\Psi_2) - \sum_{n\in\mathbb{Z}} |c_n|^2 c_n \hat{\psi}_n^3 \right).$$

Note that the correction term Ψ_1 provides the normal form transformation that removes the singular term $\epsilon^{-1/2}\mu^{-1/2}G(x)\sum_{n\in\mathbb{Z}}|c_n|^2 c_n \hat{\psi}_n^3$ from the residual equation.

Orthogonal projections to $\{\hat{\psi}_n\}_{n\in\mathbb{Z}}$ truncated at the leading-order terms as $\mu \to 0$ result in the quintic DNLS equation (1.4) with the same expression for α as in (2.6) and the following expression for χ:

$$\chi = 3\epsilon^{-1/2} \int_{\mathbb{R}} G(x) \hat{\psi}_0^3(x) \hat{\varphi}_0(x) \mathrm{d}x, \tag{2.11}$$

provided that

$$G(x) \left(|\Psi_0|^2 \Psi_0 - \sum_{n\in\mathbb{Z}} |c_n|^2 c_n \hat{\psi}_n^3 \right) = G(x) \sum_{(n_1,n_2,n_3)\in\mathbb{Z}^3 \setminus (n,n,n)} c_{n_1} \bar{c}_{n_2} c_{n_3} \hat{\psi}_{n_1} \hat{\psi}_{n_2} \hat{\psi}_{n_3} \tag{2.12}$$

is smaller than $\mathcal{O}(\epsilon^{1/2}\mu)$. The latter condition is proved in Appendix B.

We will now show that χ is bounded and nonzero as $\epsilon \to 0$. First, we note that if $G(x)$ is odd and $\hat{\psi}_0(x)$ is even on $\mathbb{R}$, then $\hat{\varphi}_0(x)$ is odd on $\mathbb{R}$, so that the integral in (2.11) is generally nonzero. Moreover, using the inhomogeneous equation (2.9), we infer that

$$\chi = -3\langle (L - \hat{E}_0)\hat{\varphi}_0, \hat{\varphi}_0 \rangle, \tag{2.13}$$

so that $\chi < 0$ for the lowest band of L, since $(L - \hat{E}_0)$ is positive definite if $\hat{E}_0$ is at the bottom of the spectrum of L in the limit $\epsilon \to 0$. To show that χ is bounded as $\epsilon \to 0$, we can use the Gaussian approximation (A.5) from Appendix A and find solutions of the inhomogeneous equation (2.9) near $x = 0$ in the form

$$\hat{\varphi}_0(x) \sim -\frac{\epsilon^{1/2} G'(0)}{8(\pi\epsilon)^{3/4}} x e^{-\frac{3x^2}{2\epsilon}}, \quad \text{near } x = 0. \tag{2.14}$$

As a result,

$$\chi \sim -\frac{(G'(0))^2}{16\sqrt{3}\pi}, \tag{2.15}$$

and we see that χ is bounded and nonzero as $\epsilon \to 0$ if $G'(0) \neq 0$.

Using the same standard approach from Pelinovsky and Schneider in [9], the quintic DNLS equation (1.4) is justified on a finite time interval, according to the following statement.

THEOREM 2 *Assume that* $V(x)$ *and* $G(x)$ *are given by* (1.3) *and* (2.1), $G'(0)\neq 0$, *and* μ *is given by* (2.4). *Let* $\{c_n(T)\}_{n\in\mathbb{Z}}\in C^1(\mathbb{R}, l^1(\mathbb{Z}))$ *be a global solution of the quintic DNLS equation* (1.4) *with initial data* $\{c_n(0)\}_{n\in\mathbb{Z}}\in l_p^2(\mathbb{Z})$ *for any* $p>\frac{1}{2}$. *Let* $\Psi_0\in\mathcal{H}^1(\mathbb{R})$ *satisfy the bound*

$$\left\|\Psi_0-\epsilon^{-1/4}\mu^{1/4}\sum_{n\in\mathbb{Z}}c_n(0)\hat{\psi}_n\right\|_{\mathcal{H}^1}\leq C_0\epsilon^{-1/4}\mu^{3/4}$$

for some $C_0>0$. *There exist* $\mu_0>0$, $T_0>0$ *and* $C>0$, *such that for any* $\mu\in(0,\mu_0)$, *the GP equation* (1.2) *with initial data* $\Psi(0)=\Psi_0$ *has a solution* $\Psi(t)\in C([0,T_0/\mu],\mathcal{H}^1(\mathbb{R}))$ *satisfying the bound*

$$\forall t\in[0,T_0/\mu]:\quad \left\|\Psi(\cdot,t)-\epsilon^{-1/4}\mu^{1/4}\left(\sum_{n\in\mathbb{Z}}c_n(\mu t)\hat{\psi}_n\right)e^{-i\hat{E}_0t}\right\|_{\mathcal{H}^1}\leq C\epsilon^{-1/4}\mu^{3/4}.$$

Remark 1 Note that the results of Theorems 1 and 2 also hold for the piecewise-constant Kronig–Pennig potential $V_0(x)$ after the required minor modifications because of a different algebraic factor of ϵ in the definition of μ [8].

3. Localized solutions of reduced equations

We shall consider the stationary solutions of the quintic DNLS equation (1.4), where the coefficients α and χ are computed asymptotically for the lowest energy band of $L=-\partial_x^2+\epsilon^{-2}V_0(x)$ in the semi-classical limit $\epsilon\to 0$.

Let $c_n(T)=\phi_n e^{-i\Omega T}$ for a real parameter Ω and a real-valued sequence $\{\phi_n\}_{n\in\mathbb{Z}}$ and obtain the stationary quintic DNLS equation

$$\alpha(\phi_{n+1}+\phi_{n-1})+\chi\phi_n^5=\Omega\phi_n,\quad n\in\mathbb{Z}. \tag{3.1}$$

The hierarchy of overlapping integrals (A.3) implies that the energy band function $E(k)$ is given at the leading order by

$$E(k)\sim\hat{E}_0+2\hat{E}_1\cos(2\pi k)+\cdots.$$

Since $k=0$ is the minimal point of $E(k)$ for the lowest energy band, we have $\hat{E}_1<0$ so that $\alpha<0$ (see also (2.7), where $\alpha<0$ is computed in the limit $\epsilon\to 0$). On the other hand, representation (2.13) implies that $\chi<0$ for the lowest band (see also (2.15), where $\chi<0$ is computed for $G'(0)\neq 0$ as $\epsilon\to 0$). The semi-infinite gap corresponds to the interval $\Omega<2\alpha$.

Existence of two localized solutions of the stationary quintic DNLS equation (3.1) for any $\text{sign}(\alpha)=\text{sign}(\chi)=\text{sign}(\Omega-2\alpha)$ is proved by Qin and Xiao [18]. Both solutions are strictly positive and satisfies reversibility reductions $\phi_{-n}=\phi_n$ (site-centred soliton) and $\phi_{-n}=\phi_{n+1}$ (bond-centred soliton) for all $n\in\mathbb{Z}$. Monotonic exponential decay of the solution $\{\phi_n\}_{n\in\mathbb{Z}}$ to zero as $n\to\pm\infty$ was shown in Theorem 1.1 of [19] (where the cubic DNLS equation was considered without loss of generality). For the semi-infinite gap, we have shown above that α and χ have equal *negative* sign, so that a localized solution of the stationary quintic DNLS equation (3.1) exists in the semi-infinite gap for $\Omega<2\alpha$.

Consider the stationary GP equation

$$-\Phi''(x) + V(x)\Phi(x) + G(x)\Phi^3(x) = \omega\Phi(x), \quad x \in \mathbb{R}, \tag{3.2}$$

which is derived from the GP equation (1.2) from $\Psi(x,t) = \Phi(x)e^{-i\omega t}$. Persistence analysis in [8] gives the existence of small-amplitude gap solitons in the stationary GP equation (3.2).

THEOREM 3 *Let $V(x)$ and $G(x)$ satisfy* (1.3) *and* (2.1), $G'(0) \neq 0$, *and μ is given by* (2.4). *Let $\{\phi_n\}_{n\in\mathbb{Z}} \in l^1(\mathbb{Z})$ be a ground state of the stationary quintic DNLS equation* (3.1) *for $\Omega < 2\alpha$. There exist $\mu_0 > 0$ and $C > 0$, such that for any $\mu \in (0, \mu_0)$, the stationary GP equation* (3.2) *with $\omega = \hat{E}_0 + \mu\Omega$ has a solution $\Phi \in \mathcal{H}^1(\mathbb{R})$ satisfying the bound*

$$\left\| \Phi - \epsilon^{-1/4}\mu^{1/4}\left(\sum_{n\in\mathbb{Z}} \phi_n \hat{\psi}_n\right) \right\|_{\mathcal{H}^1} \leq C\epsilon^{-1/4}\mu^{3/4}.$$

Moreover, $\phi(x)$ decays to zero exponentially fast as $|x| \to \infty$.

Remark 2 One can also prove the existence of large-amplitude gap solitons in the stationary GP equation (3.2) with potentials (1.3) using the Lyapunov–Schmidt reduction method. See Sivan et al. [20] for an example of this technique for the GP equation with a periodic linear potential $V(x)$ and a constant nonlinearity coefficient.

To summarize, from Theorem 3, we predict the existence of gap solitons in the semi-infinite gap for any even $V(x)$ and odd $G(x)$ with $G'(0) \neq 0$. To illustrate the existence numerically, we solve the GP equation by using the so-called imaginary time method [21]. As approximations of localized solutions evolve along the imaginary time, iterations converge to the ground state of the stationary GP equation (3.2).

We have developed a Fourier pseudospectral scheme for the discretization of the spatial derivatives combined with a split-step scheme for iterations in the imaginary time, see implementation of this method by Montesinos and Pérez-García [22]. In this method, solutions of

$$\partial_t U(x,t) = (A + B)U$$

with

$$A = -\partial_{xx}, \quad B = V(x) + G(x)|U|^2$$

are approximated from exact solutions of the problems $\partial_t U = AU$ and $\partial_t U = BU$. By using the symmetric (second-order) split-step method, whose equation is

$$U(x, t+\tau) = e^{\tau A/2}e^{\tau B}e^{\tau A/2}U(x,t) + \mathcal{O}(\tau^3), \tag{3.3}$$

we calculate a localized solution of the stationary GP equation (3.2) as $t \to \infty$. Figure 1 shows the branch of gap solitons bifurcating to the semi-infinite gap (Figure 1a) and a particular profile of the localized solution (Figure 1b) that corresponds to the point on the solution branch on the left.

We note that the numerical scheme we have used has many advantages. First, it is more accurate than finite-difference numerical methods. Second, the Fourier

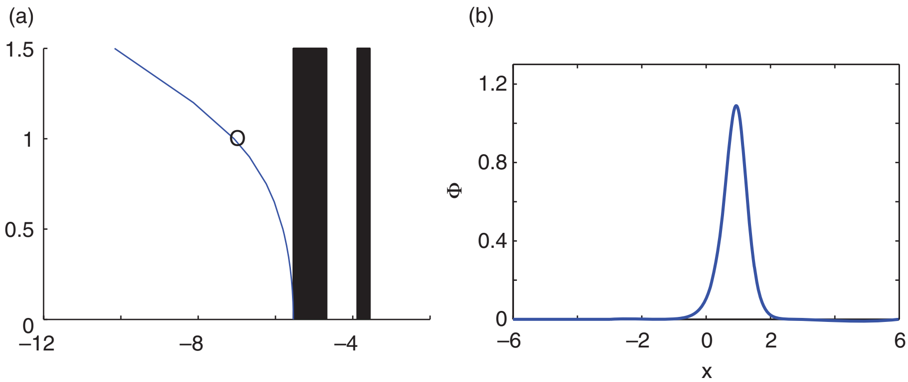

Figure 1. The solution family of gap solitons for $G_0 = -10$ and $V_0 = 6$ in (1.6): The L^2-norm N versus ω (a) and the spatial profile of gap soliton corresponding to marked point with a black circle (b).

transform can be computed by using the fast Fourier transform. Finally, the L^2-norm of the localized solutions is preserved during the time iterations so that the L^2-norm of a gap soliton along the solution branch can be fixed by the starting approximation.

In the end, we note that the existence of localized solutions in the stationary GP equation (3.2) for any smooth 2π-periodic even $V(x)$ and odd $G(x)$ in the semi-infinite gap of L can be proved using the variational theory by a modification of arguments in [5]. This modification is a subject of an ongoing work [6]. Numerical evidences of the existence of gap solitons in the semi-infinite gap for sign-varying nonlinearity coefficients can be found in [14,15].

4. Discussion of the generalized DNLS equation with intersite cubic terms

Let us compare the main result of Section 3 with the prediction based on the stationary generalized DNLS equation considered by Abdullaev et al. [4]. For the case of odd nonlinearity coefficient $G(x)$, this stationary equation is written in the form

$$\alpha(\phi_{n+1} + \phi_{n-1}) + \gamma(3\phi_n^2(\phi_{n+1} - \phi_{n-1}) - \phi_{n+1}^3 + \phi_{n-1}^3) = \Omega\phi_n, \quad n \in \mathbb{Z}, \tag{4.1}$$

where α is the same as in (3.1) and γ is proportional to the overlapping integral (B.3). Note that the cubic term in (4.1) is slightly different from the one in (1.1), the latter equation holds for even nonlinearity coefficient $G(x)$ [4]. We also note that $\beta = \delta = 0$, according to (2.10) and (B.2). While we are not able to prove that the stationary DNLS equation (4.1) admits no localized solutions for any signs of α and γ, we can simplify the problem in the slowly varying approximation, which describes the small-amplitude localized mode, if it exists. To this end, we assume that the following expansion makes sense

$$\phi_{n\pm1} = \phi(x_n) \pm h\phi'(x_n) + \frac{1}{2}h^2\phi''(x_n) + \mathcal{O}(h^3),$$

where $x_n = hn$, $n \in \mathbb{Z}$ and apply the scaling

$$\alpha = 2h\hat{\alpha}, \quad \Omega - 2\alpha = 2h^3\hat{\Omega}.$$

At the leading order, the difference equation (4.1) becomes the second-order differential equation

$$\hat{\alpha}\phi''(x) - \gamma\phi'(x)\left[(\phi'(x))^2 + 3\phi(x)\phi''(x)\right] = \hat{\Omega}\phi(x), \quad x \in \mathbb{R}, \tag{4.2}$$

which has the first integral

$$I = \frac{1}{2}\hat{\alpha}(\phi'(x))^2 - \gamma\phi(x)(\phi'(x))^3 - \frac{1}{2}\hat{\Omega}\phi^2(x) = \text{const}.$$

We note that $I = 0$ for localized solutions and that no turning point $x_0 \in \mathbb{R}$ with $\phi(x_0) > 0$ and $\phi'(x_0) = 0$ exists. As a result, the trajectory departing from the critical point $(\phi, \phi') = (0, 0)$ in the first quadrant of (ϕ, ϕ') remains in the first quadrant and goes to infinity. As a result, no classical localized solutions of the differential equation (4.2) exist. Thus, we have the following result.

Proposition 1 *Stationary generalized DNLS equation* (4.1) *for any coefficients* α, γ *and* Ω *admits no localized solutions in the slowly varying approximation.*

We conclude that the stationary generalized DNLS equation (1.1) gives the *opposite* (*wrong*) conclusion to the bifurcation problem of localized solutions in the semi-infinite gap, compared to the stationary quintic DNLS equation (3.1).

It is even more problematic to interpret the modification of the generalized DNLS equation (1.1) by Smerzi and Trombettoni [1], where the onsite cubic nonlinear term $\beta|c_n|^2 c_n$ was replaced by $\beta|c_n|^{2p} c_n$ with $p \le 2$. If $\beta \neq 0$, the justification of the cubic DNLS equation (2.5) in Theorem 1 leaves no hope to have $p < 2$ in the generalized DNLS equation and to account the intersite cubic nonlinear terms at the same order as the onsite cubic nonlinear terms. Thus, we have to conclude that the generalized DNLS equations considered in [1,4] (and implicitly in [2,3]) are invalid for potential $V(x)$ in (2.1) in the tight-binding approximation as $\epsilon \to 0$.

5. Reductions to the CNLS equation

Let us now consider the potential $V(x)$ in the GP equation (1.2) without assumption (2.1). Spectral bands are generally of a finite size, so that we can simplify the GP equation (1.2) if the bound state has small amplitude near the band edge. This asymptotic reduction leads to the CNLS equation.

To give main details, let E_0 be the lowest band edge of operator $L = -\partial_x^2 + V(x)$ corresponding to the 2π-periodic L^2-normalized eigenfunction $\Psi_0 \in L^2_{\text{per}}(0, 2\pi)$. Since the second solution of $L\Psi = E_0\Psi$ is linearly growing, the subspace $\text{Ker}(L - E_0 I) \subset L^2_{\text{per}}(0, 2\pi)$ is one-dimensional. Looking at the Fredholm alternative condition for the inhomogeneous equation

$$-\Psi_1''(x) + V(x)\Psi_1(x) - E_0\Psi_1(x) = 2\Psi_0'(x), \tag{5.1}$$

we infer that there exists a unique 2π-periodic function $\Psi_1 \in L^2_{\text{per}}(0, 2\pi)$ in the orthogonal complement of $\text{Ker}(L - E_0 I)$. If $V(x)$ is even on $\mathbb{R}$, then $\Psi_0(x)$ is even and

$\Psi_1(x)$ is odd on $\mathbb{R}$. In addition, if $G(x)$ is an odd 2π-periodic function, there exists a unique odd 2π-periodic solution of the inhomogeneous equation

$$-\Psi_2''(x) + V(x)\Psi_2(x) - E_0\Psi_2(x) = -G(x)\Psi_0^3(x), \tag{5.2}$$

which also lies in the orthogonal complement of $\mathrm{Ker}(L - E_0 I)$. Equipped with these facts, we are looking for an asymptotic solution of the GP equation (1.2) using the decomposition

$$\begin{aligned}\Psi(x,t) = \varepsilon^{1/2}\big(&A(X,T)\Psi_0(x) + \varepsilon\big(A_X(X,T)\Psi_1(x) + |A(X,T)|^2 A(X,T)\Psi_2(x)\big)\\ &+ \varepsilon^2\tilde{\Psi}(x,t)\big)e^{-iE_0 t},\end{aligned}$$

where ε is a small parameter, $X = \varepsilon x$ and $T = \varepsilon^2 t$ are slow variables, and $\tilde{\Psi}(x,t)$ satisfies the time evolution equation

$$\begin{aligned}i\partial_t\tilde{\Psi} = {} & (L - E_0)\tilde{\Psi} - iA_T\Psi_0 - \varepsilon\big(A_{XT}\Psi_1 + (|A|^2A)_T\Psi_2\big)\\ & - A_{XX}\big(\Psi_0 + 2\Psi_1'\big) - 2(|A|^2A)_X\Psi_2' - \varepsilon\big(A_{XXX}\Psi_1 + (|A|^2A)_{XX}\Psi_2\big)\\ & + G(x)\varepsilon^{-1}\big(|A\Psi_0 + \varepsilon\big(A_X\Psi_1 + |A|^2A\Psi_2\big) + \varepsilon^2\tilde{\Psi}|^2\\ & \times (A\Psi_0 + \varepsilon\big(A_X\Psi_1 + |A|^2A\Psi_2\big) + \varepsilon^2\tilde{\Psi}) - |A|^2A\Psi_0^3\big).\end{aligned}$$

Projecting the right-hand side to Ψ_0 and truncating at the leading-order terms, we obtain the CNLS equation

$$iA_T = \alpha A_{XX} + \chi|A|^4A + \gamma\big(|A|^2A\big)_X, \tag{5.3}$$

where

$$\begin{aligned}\alpha &= -1 - 2\int_0^{2\pi}\Psi_1'(x)\Psi_0(x)\mathrm{d}x,\\ \chi &= 3\int_0^{2\pi}G(x)\Psi_0^3(x)\Psi_2(x)\mathrm{d}x,\\ \gamma &= -2\int_0^{2\pi}\Psi_2'(x)\Psi_0(x)\mathrm{d}x + \int_0^{2\pi}G(x)\Psi_0^3(x)\Psi_1(x)\mathrm{d}x.\end{aligned}$$

Justification of the generalized CNLS equation (5.3) can be developed similarly to the work of Busch et al. [10]. While it may seem that the generalized CNLS equation (5.3) contains both the quintic and the cubic derivative terms, we obtain that

$$\begin{aligned}\gamma &= \int_0^{2\pi}\big(-2\Psi_2'(x)\Psi_0(x) + G(x)\Psi_0^3(x)\Psi_1(x)\big)\mathrm{d}x\\ &= -\int_0^{2\pi}\big(2\Psi_2'(x)\Psi_0(x) + \Psi_1(x)\big(-\partial_x^2 + V(x) - E_0\big)\Psi_2(x)\big)\mathrm{d}x\\ &= -\int_0^{2\pi}\big(2\Psi_2(x)\Psi_0'(x) + \Psi_2(x)\big(-\partial_x^2 + V(x) - E_0\big)\Psi_1(x)\big)\mathrm{d}x = 0.\end{aligned}$$

Therefore, the generalized CNLS equation (5.3) is just the quintic CNLS equation

$$iA_T = \alpha A_{XX} + \chi|A|^4A. \tag{5.4}$$

For stationary solutions with $A(X,T) = a(X)e^{-i\Omega T}$, where Ω and $a(X)$ are real-valued, we obtain the stationary quintic nonlinear Schrödinger (NLS) equation in the form

$$\alpha a''(X) + \chi a^5(X) = \Omega a(X), \quad X \in \mathbb{R}. \tag{5.5}$$

Similar to the case in the tight-binding approximation, we note that $\alpha < 0$ and $\chi < 0$ for the semi-infinite gap since $\alpha = -\frac{1}{2}E''(0) < 0$, where $E(k)$ is the energy band function for the lowest energy band, and

$$\chi = 3\int_0^{2\pi} G(x)\Psi_0^3(x)\Psi_2(x)\mathrm{d}x = -3\int_0^{2\pi} \Psi_2(x)\left(-\partial_X^2 + V(x) - E_0\right)\Psi_2(x)\mathrm{d}x < 0.$$

The stationary quintic NLS equation (5.5) has a positive definite soliton for $\mathrm{sign}(\alpha) = \mathrm{sign}(\chi)$ with $\mathrm{sign}(\Omega) = \mathrm{sign}(\alpha)$, that is for $\Omega < 0$ in the semi-infinite gap.

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Appendix A: Review of the semi-classical analysis for the linear Schrödinger equation with a periodic potential

Let $\Psi(x;k)$ be the Bloch function of

$$L\Psi(x;k) = E(k)\Psi(x;k), \quad L = -\partial_x^2 + \epsilon^{-2} V_0(x) \tag{A1}$$

for the lowest energy band function $E(k)$. It is known (see review in [8]) that $E(k)$ and $\Psi(x,k)$ satisfy

$$E(k) = E(k+1) = E(-k), \quad k \in \mathbb{R}$$

and

$$\Psi(x;k) = e^{-2\pi k i}\Psi(x+2\pi;k) = \Psi(x;k+1) = \bar{\Psi}(x;-k), \quad x \in \mathbb{R}, \quad k \in \mathbb{R},$$

so that one can define the Fourier series decompositions

$$E(k) = \sum_{n \in \mathbb{Z}} \hat{E}_n e^{2\pi n k i}, \quad \Psi(x;k) = \sum_{n \in \mathbb{Z}} \hat{\psi}_n(x) e^{2\pi n k i},$$

with real-valued Fourier coefficients satisfying the reduction

$$\hat{E}_n = \hat{E}_{-n}, \quad \hat{\psi}_n(x) = \hat{\psi}_0(x - 2\pi n), \quad n \in \mathbb{Z}.$$

Functions $\{\hat{\psi}_n(x)\}_{n\in\mathbb{Z}}$ are referred to as the Wannier functions. For the lowest energy band, these functions form an orthonormal basis in a subspace of $L^2(\mathbb{R})$ associated with the lowest energy band, enjoy an exponential decay to zero as $|x|\to\infty$ and satisfy the system of differential equations

$$\left(L-\hat{E}_0\right)\hat{\psi}_0(x)=\sum_{n\geq 1}\hat{E}_n\left(\hat{\psi}_n(x)+\hat{\psi}_{-n}(x)\right),\quad x\in\mathbb{R}. \tag{A2}$$

Thanks to the orthogonality and normalization of the Wannier functions, we infer that $\hat{E}_n$ can be computed from the overlapping integrals

$$\hat{E}_n=\langle L\hat{\psi}_0,\hat{\psi}_n\rangle=\int_{\mathbb{R}}\left[\hat{\psi}_0'(x)\hat{\psi}_n'(x)+\epsilon^{-2}V_0(x)\hat{\psi}_0(x)\hat{\psi}_n(x)\right]\mathrm{d}x,\quad n\in\mathbb{N}. \tag{A3}$$

For the semi-infinite gap and for even potentials, Wannier functions $\{\hat{\psi}_n(x)\}_{n\in\mathbb{Z}}$ are strictly positive and even on $\mathbb{R}$. It is proved with the standard technique in the semi-classical limit $\epsilon\to 0$ (see review in [23]) that the Wannier function $\hat{\psi}_0(x)$ can be approximated near $x=0$ by the normalized Gaussian eigenfunction of

$$\left(-\partial_x^2+\frac{x^2}{\epsilon^2}\right)\psi_0(x)=\frac{1}{\epsilon}\psi_0(x),\quad x\in\mathbb{R},$$

or explicitly,

$$\psi_0(x)=\frac{1}{(\pi\epsilon)^{1/4}}e^{-\frac{x^2}{2\epsilon}},\quad x\in\mathbb{R}. \tag{A4}$$

This approximation suggests that

$$\hat{E}_0\sim\frac{1}{\epsilon},\quad \hat{\psi}_0(x)\sim\psi_0(x),\quad \text{near } x=0, \tag{A5}$$

where we have used the notation $A(\epsilon)\sim B(\epsilon)$ for two functions of ϵ near $\epsilon=0$ to indicate that $A(\epsilon)/B(\epsilon)\to 1$ as $\epsilon\to 0$. To obtain approximations for the overlapping integrals (A.3), one need to proceed with the Wentzel–Kramers–Brillouin (WKB) solution

$$\hat{\psi}_0(x)\sim A(x)e^{-\frac{1}{\epsilon}\int_0^x S(x')\mathrm{d}x'},\quad x\in(0,2\pi), \tag{A6}$$

where

$$S(x)=\sqrt{V_0(x)},$$
$$A(x)=\frac{1}{(\pi\epsilon)^{1/4}}\exp\left[\int_0^x\frac{1-S'(x')}{2S(x')}\mathrm{d}x'\right],\quad x\in(0,2\pi).$$

The WKB solution (A6) is derived by neglecting the term $A''(x)$ in the left-hand side of (A2) and by dropping the right-hand side of (A2) using the hierarchy of overlapping integrals in

$$\cdots\ll|\hat{E}_2|\ll|\hat{E}_1|\ll|\hat{E}_0|. \tag{A7}$$

In addition, to derive the explicit expression for $A(x)$ we have replaced $\hat{E}_0$ by $1/\epsilon$ and used the matching condition of $\hat{\psi}_0(x)$ with $\psi_0(x)$ as $x\downarrow 0$. Note that the expression for $A(x)$ diverges as $x\uparrow 2\pi$.

Using the explicit formulas and the symmetry of $\hat{\psi}_0(x)$ on $\mathbb{R}$, the first overlapping integral is computed as follows:

$$\begin{aligned}\hat{E}_1&=2\int_{-\infty}^{\pi}\hat{\psi}_0(x)\left(-\partial_x^2+\epsilon^{-2}V_0(x)-\hat{E}_0\right)\hat{\psi}_0(x-2\pi)\mathrm{d}x\\&=4\hat{\psi}_0(\pi)\hat{\psi}_0'(\pi)+2\int_{-\infty}^{\pi}\hat{\psi}_0(x-2\pi)\left(-\partial_x^2+\epsilon^{-2}V_0(x)-\hat{E}_0\right)\hat{\psi}_0(x)\mathrm{d}x.\end{aligned}$$

Neglecting the integral (again using smallness of the right-hand side of (A.2) on $(-\infty,-\pi]$) and substituting the WKB solution (A6) at $x=\pi$, we infer that the leading order of the first overlapping integral is given by

$$\hat{E}_1 \sim 4\hat{\psi}_0(\pi)\hat{\psi}_0'(\pi) = -\frac{4\sqrt{V_0(\pi)}}{\pi^{1/2}\epsilon^{3/2}}\exp\left(-\frac{2}{\epsilon}\int_0^\pi \sqrt{V_0(x)}\mathrm{d}x + \int_0^\pi \frac{1-S'(x)}{S(x)}\mathrm{d}x\right). \tag{A8}$$

For instance, if $V_0(x)=2(1-\cos(x))$, then

$$S(x) = 2\sin\left(\frac{x}{2}\right), \quad A(x) = \frac{1}{(\pi\epsilon)^{1/4}\cos\left(\frac{x}{4}\right)}, \quad x\in(0,2\pi),$$

so that

$$\hat{E}_1 \sim -\frac{16}{\pi^{1/2}\epsilon^{3/2}}e^{-\frac{8}{\epsilon}}.$$

Similarly, one can establish the hierarchy of other overlapping integrals in (A7). See Helffer [17] for rigorous justification of the above WKB solutions.

To deal with nonlinear terms, we compute the integral involving $G(x)\hat{\psi}_0^4(x)$ as $\epsilon\to 0$. This integral can be computed with the use of the Gaussian approximation (A4) and (A5), using the fast decay of $\hat{\psi}_0(x)$ on $\mathbb{R}$ and the smoothness of $G(x)$ on $\mathbb{R}$:

$$\int_{\mathbb{R}} G(x)\hat{\psi}_0^4(x)\mathrm{d}x \sim \frac{1}{\pi\epsilon}\int_{\mathbb{R}} G(x)e^{-\frac{2x^2}{\epsilon}}\mathrm{d}x \sim \frac{1}{(2\pi\epsilon)^{1/2}}G(0). \tag{A9}$$

The overlapping integrals involving homogeneous quartic powers of $\hat{\psi}_0(x)$, $\hat{\psi}_0(x-2\pi)$, etc., are much smaller compared to the integral (A9), again according to the fast decay of $\hat{\psi}_0(x)$ on $\mathbb{R}$.

Appendix B: Nonlinear overlapping integrals

The largest overlapping integrals from the cubic term (2.12) are given by

$$\int_{\mathbb{R}} G(x)\hat{\psi}_0^3(x)\hat{\psi}_0(x-2\pi)\mathrm{d}x, \quad \int_{\mathbb{R}} G(x)\hat{\psi}_0^2(x)\hat{\psi}_0^2(x-2\pi)\mathrm{d}x. \tag{B1}$$

We need to show that these largest terms are smaller than $\epsilon^{1/2}\mu$.

First, we note that if $G(x)$ is a smooth, 2π-periodic and an odd function, then $G(x)$ is also odd with respect to the point $x=\pi$, so that

$$\int_{\mathbb{R}} G(x)\hat{\psi}_0^2(x)\hat{\psi}_0^2(x-2\pi)\mathrm{d}x = 0. \tag{B2}$$

To consider the other nonzero integral in (B1), we write

$$\int_{\mathbb{R}} G(x)\hat{\psi}_0^3(x)\hat{\psi}_0(x-2\pi)\mathrm{d}x = \left(\int_{-\infty}^{\pi} + \int_{\pi}^{\infty}\right)G(x)\hat{\psi}_0^3(x)\hat{\psi}_0(x-2\pi)\mathrm{d}x. \tag{B3}$$

The second integral on $[\pi,\infty)$ is much smaller than the first integral on $(-\infty,\pi]$, according to the faster decay of $\hat{\psi}_0^3(x)$ compared to $\hat{\psi}_0(x)$ on $\mathbb{R}$. As a result, we deal only with the first integral, which we rewrite as follows:

$$\begin{aligned}
\int_{-\infty}^{\pi} G(x)\hat{\psi}_0^3(x)\hat{\psi}_0(x-2\pi)\mathrm{d}x &= -\epsilon^{1/2}\int_{-\infty}^{\pi}\hat{\psi}_0(x-2\pi)\left(-\partial_x^2+\epsilon^{-2}V_0(x)-\hat{E}_0\right)\hat{\varphi}_0(x)\mathrm{d}x \\
&= \epsilon^{1/2}\left[\hat{\psi}_0(\pi)\hat{\varphi}_0'(\pi)+\hat{\psi}_0'(\pi)\hat{\varphi}_0(\pi)\right] \\
&\quad - \epsilon^{1/2}\int_{-\infty}^{\pi}\hat{\varphi}_0(x)\left(-\partial_x^2+\epsilon^{-2}V_0(x)-\hat{E}_0\right)\hat{\psi}_0(x-2\pi)\mathrm{d}x,
\end{aligned} \tag{B4}$$

where we recall again that $\hat{\psi}_0(x)$ is even on $\mathbb{R}$. In view of Equation (A2), we have

$$\begin{aligned}
&\int_{-\infty}^{\pi} \hat{\varphi}_0(x)\Big(-\partial_x^2 + \epsilon^{-2}V_0(x) - \hat{E}_0\Big)\hat{\psi}_0(x-2\pi)\mathrm{d}x \\
&= \sum_{n\geq 1} \hat{E}_n \int_{-\infty}^{\pi} \hat{\varphi}_0(x)\Big(\hat{\psi}_{n+1}(x) + \hat{\psi}_{-n+1}(x)\Big)\mathrm{d}x \\
&\sim \hat{E}_1 \int_{-\infty}^{\pi} \hat{\varphi}_0(x)\hat{\psi}_0(x)\mathrm{d}x = -\hat{E}_1 \int_{\pi}^{\infty} \hat{\varphi}_0(x)\hat{\psi}_0(x)\mathrm{d}x,
\end{aligned}$$

where the last equality is due to the fact that $\hat{\psi}_0(x)$ is even and $\hat{\varphi}_0(x)$ is odd on $\mathbb{R}$.

Thanks to the fast decay of $\hat{\psi}_0(x)$ and $\hat{\varphi}_0(x)$ on $\mathbb{R}$, the second term in (B4) becomes smaller than $\epsilon^{1/2}\hat{E}_1 = \epsilon^{1/2}\mu\alpha$, where α is given by (2.6).

Boundary values of $\hat{\psi}_0(x)$, $\hat{\varphi}_0(x)$ and their derivatives at $x=\pi$ in the first term in (B4) can again be computed from the WKB solutions for $\hat{\psi}_0(x)$ and $\hat{\varphi}_0(x)$.

For solutions of the inhomogeneous equation (2.9), we substitute

$$\hat{\varphi}_0(x) \sim B(x)e^{-\frac{3}{\epsilon}\int_0^x S(x')\mathrm{d}x'}, \quad x \in (0, 2\pi),$$

where $S(x) = \sqrt{V_0(x)}$ and $B(x)$ satisfies the first-order differential equation

$$\epsilon(6S(x)B'(x) + 3S'(x)B(x) - B(x)) - 8S^2(x)B(x) = -\epsilon^{3/2}G(x)A^3(x),$$

where the term $B''(x)$ is neglected and $\hat{E}_0 \sim 1/\epsilon$ is used. Solving the differential equation with the integration factor, we obtain

$$B(x) = \frac{C(x)}{S^{1/3}(x)}\exp\left(\frac{4}{3\epsilon}\int_0^x S(x')\mathrm{d}x' + \frac{1}{6}\int_0^x \frac{1-S'(x')}{S(x')}\mathrm{d}x'\right), \quad x \in (0, 2\pi),$$

with

$$C(x) = -\frac{\epsilon^{1/2}}{6}\int_0^x \frac{G(x')A^3(x')}{S^{1/3}(x')}\exp\left(-\frac{4}{3\epsilon}\int_0^{x'} S(x'')\mathrm{d}x'' - \frac{1}{6}\int_0^{x'} \frac{1-S'(x'')}{S(x'')}\mathrm{d}x''\right)\mathrm{d}x'.$$

Using the Laplace method for computing integrals, we obtain a correct behaviour of $\hat{\varphi}_0(x)$ near $x=0$ that matches the previous calculation (2.14):

$$\begin{aligned}
\hat{\varphi}_0(x) &\sim -\frac{\epsilon^{1/2}G'(0)}{6(\pi\epsilon)^{3/4}x^{1/3}}e^{-\frac{3x^2}{2\epsilon}}\int_0^x y^{1/3}e^{-\frac{2}{3\epsilon}(y^2-x^2)}\mathrm{d}y \\
&\sim -\frac{\epsilon^{1/2}G'(0)}{8(\pi\epsilon)^{3/4}}xe^{-\frac{3x^2}{2\epsilon}}, \quad \text{near } x=0.
\end{aligned}$$

As a result, we have

$$\epsilon^{1/2}\Big[\hat{\psi}_0(\pi)\hat{\varphi}_0'(\pi) + \hat{\psi}_0'(\pi)\hat{\varphi}_0(\pi)\Big] \sim \frac{4}{9}S^{2/3}(\pi)A(\pi)\exp\left(-\frac{8}{3\epsilon}\int_0^{\pi} S(x)\mathrm{d}x + \frac{1}{6}\int_0^{\pi}\frac{1-S'(x)}{S(x)}\mathrm{d}x\right)C_0,$$

where

$$C_0 = \int_0^{\pi} \frac{G(x)A^3(x)}{S^{1/3}(x)}\exp\left(-\frac{4}{3\epsilon}\int_0^x S(x')\mathrm{d}x' - \frac{1}{6}\int_0^x \frac{1-S'(x')}{S(x')}\mathrm{d}x'\right)\mathrm{d}x.$$

For instance, if $V(x) = 2(1-\cos(x))$, we obtain

$$\epsilon^{1/2}\Big[\hat{\psi}_0(\pi)\hat{\varphi}_0'(\pi) + \hat{\psi}_0'(\pi)\hat{\varphi}_0(\pi)\Big] \sim \frac{4}{9\pi\epsilon}e^{-\frac{48}{3\epsilon}}\int_0^{\pi}\frac{G(x)}{\sin^{2/3}(\frac{x}{4})\cos^{10/3}(\frac{x}{4})}e^{-\frac{16}{3\epsilon}\cos(\frac{x}{2})}\mathrm{d}x,$$

which is clearly smaller than

$$\epsilon^{1/2}\mu = \frac{1}{\pi^{1/4}\epsilon}\exp\left(-\frac{2}{\epsilon}\int_0^{\pi} S(x)\mathrm{d}x\right) = \frac{1}{\pi^{1/4}\epsilon}e^{-\frac{8}{\epsilon}}.$$