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LOWER PART OF THE SPECTRUM FOR THE TWO-DIMENSIONAL SCHRÖDINGER OPERATOR PERIODIC IN ONE VARIABLE AND APPLICATION TO QUANTUM DIMERS

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We study the semiclassical asymptotic approximation of the spectrum of the two-dimensional Schrödinger operator with a potential periodic in x and increasing at infinity in y. We show that the lower part of the spectrum has a band structure (where bands can overlap) and calculate their widths and dispersion relations between energy and quasimomenta. The key role in the obtained asymptotic approximation is played by librations, i.e., unstable periodic trajectories of the Hamiltonian system with an inverted potential. We also present an effective numerical algorithm for computing the widths of bands and discuss applications to quantum dimers.

Keywords: periodic Schrödinger operator, spectrum, tunneling effect, spectral band, dispersion relation

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1. Introduction

This paper is devoted to studying the spectrum of a Schrödinger operator

$$\widehat{H} = -\frac{h^2}{2}\left(\frac{\partial^2}{\partial x^2} + \frac{\partial^2}{\partial y^2}\right) + \frac{y^2}{2} - \alpha\cos\beta x\cos(y - y_0) \tag{1}$$

in the semiclassical approximation $h \to +0$. Here, $\alpha, \beta > 0$ and $y_0 \pmod{2\pi}$ are parameters. Operator (1) serves as a simplified model for investigating quantum effects that appear in the one-dimensional motion of a two-atom molecule over the surface of a solid [1]. For brevity, we call this system a quantum dimer in what follows.

On the other hand, operator (1) provides an example of a quite simple two-dimensional quantum system whose potential is periodic in one variable and increases at infinity in the other. Such systems are insufficiently studied in the mathematical literature in contrast to systems with potentials periodic on

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a lattice (see [2]). The variables in the corresponding spectral problem do not separate, which makes the problem nontrivial, but asymptotic methods allow effectively calculating some of its spectral characteristics.

Our goal here is to study the lower part of the spectrum of $\widehat{H}$. Namely, we are interested in energies that lie near the minimum of the potential and correspond to Bloch functions in x, i.e., such that $\psi(x+2\pi/\beta, y) = e^{2\pi i q}\psi(x,y)$. The real parameter q (mod 1) is called the quasimomentum.

Operator (1) is related to quantum dimers as follows. The operator describing a quantum dimer moving on a periodic one-dimensional substrate has the form [1]

$$\widehat{\mathcal{H}} = -\frac{\hbar^2}{2m}\left(\frac{\partial^2}{\partial x_1^2} + \frac{\partial^2}{\partial x_2^2}\right) + \frac{K^2}{2}(x_2 - x_1 - l)^2 + U_0(2 - \cos kx_1 - \cos kx_2),$$

where m is the mass, K^2 is the rigidity, U_0 is the depth of the potential relief, $2\pi/k$ is the period of the substrate potential, and l is the equilibrium distance between atoms in the molecule. Using the new coordinates $x = k(x_1 + x_2)/2$ and $y = k(x_2 - x_1 - l)/2$ and the new parameters $\alpha = U_0k^2/2K^2$, $h^2 = k^4\hbar^2/8mK^2$, and $y_0 = -kl/2$ yields $\widehat{\mathcal{H}} = (K^2/k^2)\widehat{H} + 2U_0$, where $\widehat{H}$ has form (1) with $\beta = 1$.

Changing the quantum momenta (operators) $-ih\,\partial/\partial x$ and $-ih\,\partial/\partial y$ to the classical momenta p_x and p_y, we obtain the classical Hamiltonian corresponding to (1):

$$H = \frac{1}{2}(p_x^2 + p_y^2) + U(x,y), \qquad U = \frac{y^2}{2} - \alpha\cos\beta x\cos(y - y_0), \tag{2}$$

where the cylinder

$$Z = \left\{x \left(\mathrm{mod}\frac{2\pi}{\beta}\right),\ y \in \mathbb{R}\right\}$$

serves as the configuration space.

We stress that this Hamiltonian system is not integrable. Moreover, there are domains in the phase space where the behavior of its trajectories is chaotic (see [1]). Because of the well-known correspondence between classical and quantum systems, a large part of the spectrum of $\widehat{H}$ apparently has a rather complicated and irregular structure. Nevertheless, the lower part of the spectrum—the ground and weakly excited states—is very regular and consists of bands and gaps, which can be described using rather explicit asymptotic formulas with respect to the small parameter h.

The potential U near a global minimum point $(\tilde{x}, \tilde{y})$ can be approximated by the harmonic oscillator potential. This allows constructing the discrete set of points

$$E_{mn} = U_{\min} + \omega_1 h\left(\frac{1}{2} + m\right) + \omega_2 h\left(\frac{1}{2} + n\right) + O(h^2), \quad m, n \in \mathbb{Z}_+, \tag{3}$$

where $U_{\min} = U(\tilde{x}, \tilde{y})$, and ω_1 and ω_2 are the small oscillations frequencies, i.e., the square roots of the eigenvalues of the second derivative matrix $d^2U(\tilde{x}, \tilde{y})$.

Because of the periodic properties of the potential, the spectrum of operator (1) is continuous, and points (3) specify the positions of spectral bands. The widths of these bands are exponentially small as $h \to 0$, and the harmonic oscillator approximation cannot describe them: tunnel effects should be taken into account. The points where the global minimum of U is attained depend on the parameters α, β, and y_0. Hence, the spectral band structure of operator (1) also depends on these parameters.

Proposition 1. *The global minimum of the function $U(x,y)$ on the cylinder Z is attained at either one or two points. Namely, we have two cases.*

Case 1. *If $|y_0| < \pi/2$, then there is a unique global minimum point $x = 0$, $y = y_*$, where y_* is the solution of the equation $y + \alpha\sin(y - y_0) = 0$ closest to zero. If $\pi/2 < |y_0| \le \pi$, then there is a unique global*

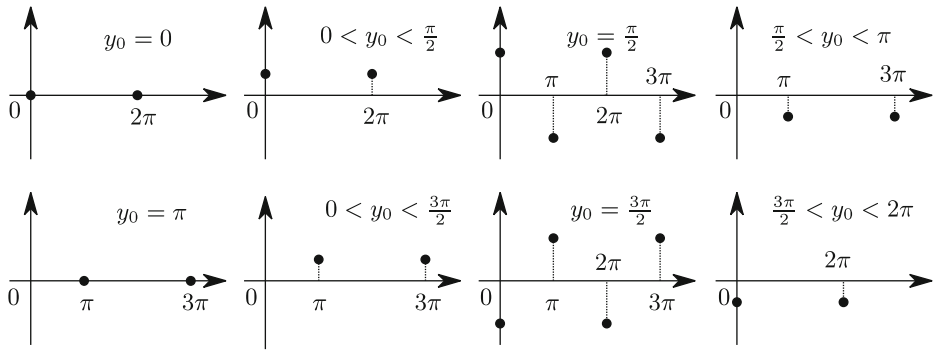


Fig. 1. The points of the global minimum for U: the horizontal axis is the x axis and the vertical axis is the y axis.

minimum point $x = \pi/\beta$, $y = y_*$, where y_* is the solution of the equation $y - \alpha \sin(y - y_0) = 0$ closest to zero.

Case 2. *If $y_0 = \pi/2$ or $y_0 = -\pi/2$), then there are two global minimum points $(0, y_*)$ and $(\pi/\beta, -y_*)$, where y_* is the solution of the respective equation $y - \alpha \cos y = 0$ or $y + \alpha \cos y = 0$ closest to zero.*

We present the proof of Proposition 1 in Appendix A.

Remark 1. Obviously, Case 1 is generic. In both cases, the potential has an axial symmetry:

$$U(-x, y) = U(x, y).$$

In Case 2, there is an additional central symmetry $U(\pi - x, -y) = U(x, y)$. We also note the special Case 0, where $y_0 = 0$ or $y_0 = \pi$.

Proposition 1 is illustrated in Fig. 1 (for $\beta = 1$).

It turns out that the structure of the lower part of the spectrum is as follows. In Case 1, a spectral band consisting of energies E corresponding to Bloch functions in the x variable is associated with each *quantum vector* $(m, n) \in \mathbb{Z}^2_+$. Moreover, each quasimomentum q corresponds to a unique energy E, and the function $E = E_{mn}(q)$, called the *dispersion relation*, is hence well defined. In Case 2, two analogous bands are associated with each quantum vector. This fact can be simply explained by considering an example with separated variables:

$$\widetilde{U} = \alpha(1 - \cos x) + V(y). \tag{4}$$

In Sec. 2.2, we study two cases: $V = y^2/2$ (Case A) and $V = (y^2 - a^2)^2/2$ (Case B), which are similar to the respective Cases 1 and 2. We easily see that each quantum vector is associated with one band in Case A and with two bands in Case B.

The problem of calculating the widths of bands and dispersion relations is by no means trivial, and we here present two approaches for solving it. The mathematically rigorous approach reduces the question to a problem with a potential having a few wells on the cylinder, to which the Helffer–Sjöstrand theory is already applicable (see [3]). This approach works in the case with rational quasimomenta q. The other approach [4], which is a multidimensional generalization of the method described in [5], [6], allows deriving correct formulas on the physical level of rigor (we call it the Herring method or approach in what follows). At the same time, the latter approach seems useful in view of its simplicity. We use it for a "hand-waving" explanation of the form of the dispersion relation in Case 1.

We note that the considered periodic problem is close to the spectrum-splitting problem for a potential with two symmetric wells studied in detail in [3], [7]–[11]. In both cases, studying the semiclassical exponentially small (or tunnel) effects leads to the Hamiltonian system $H = (p_x^2 + p_y^2)/2 - U(x, y)$ with an "inverted" potential. An important role is played by special trajectories of this Hamiltonian system, called instantons and librations. In the one-dimensional case, an instanton is a separatrix or doubly asymptotic motion corresponding to a minimum of the potential $U(x, y)$, and a libration is a periodic trajectory close to an instanton. Analogous objects arise in the multidimensional—in particular, two-dimensional—case, but their existence is already not so obvious (see Sec. 3 below).

The asymptotic formula for splitting of the ground-state eigenvalues in the symmetric double-well problem can be written in two forms: "in terms of an instanton" [8], [9] or "in terms of a libration" [10], [11]. The mechanical action along the corresponding instanton or libration is written in the exponent. The preexponential factor is expressed in terms of the motions transverse to the instanton or libration. It is important that although the two formulas are equivalent (passing from one to the other is a problem in classical mechanics), the form of the preexponential factor in the expression "in terms of an instanton" is significantly worse. It invokes a scattering problem for the variational equation, a boundary value problem with conditions at infinity. Using such a formula in practice leads to cumbersome computations. In the case of very large dimensions, this method is generally inapplicable because of the so-called determinant problem (see [12]). In view of its bulkiness (especially in the multidimensional case), the splitting formula "in terms of an instanton" is not written here (it can be found in [8]).

On the other hand, the splitting formula "in terms of a libration" [10], [11] is significantly simpler:

$$\Delta E = b\frac{\omega h}{\pi}e^{-S/h}(1 + O(h)).$$

Here, S is the action along a certain libration called a *tunnel libration*, ω is one of the harmonic oscillator frequencies, and b is a universal constant (independent of the potential). (A more precise formulation is given below.) In the one-dimensional case, the tunnel libration is just a libration corresponding to the energy of a given state. In the multidimensional case, this is no longer true, and the tunnel libration is found from an implicit equation, which involves an invariant object, the Floquet exponent of a libration. This formula is simple and esthetic, which from the physical standpoint reflects the fact that zero energy has no meaning in quantum mechanics, in contrast to the ground state energy. We also note that the similarity of this formula to the Landau–Lifshitz formula for highly excited states in a one-dimensional problem (see Problem 3 in Sect. VII.50 in [5]).

Here, we show how to write the asymptotic approximation "in terms of a libration" for the band widths and dispersion relations in the two-dimensional periodic problem. We also propose an effective numerical algorithm for practical implementation of these asymptotic approximations. Similar calculations in the double-well case were presented in [13].

This paper has the following structure. In Sec. 2, we recall well-known facts about the structure of the lower part of the spectrum of the one-dimensional Schrödinger operator and rewrite the dispersion relations for lower spectral bands "in terms of a libration." We then study the spectral structure and dispersion relations for Cases A and B. In Sec. 3, we describe instantons and librations in the two-dimensional periodic problem.

The main results are presented in Sec. 4: Theorems 3, 4, and 5 describe dispersion relations (in particular, band widths) in Cases 1 and 2.

Section 5 is devoted to computing band widths numerically. In Sec. 6, we show how to derive dispersion relations in Case 1 using the Herring approach. In Sec. 7, we explain the Helffer–Sjöstrand interaction matrix method. In Sec. 8, we prove the theorems from Sec. 4 and also derive the dispersion relations "in terms

of a libration" for the lowest band in the one-dimensional case (Theorem 1) without requiring the mirror symmetry $x \to -x$.

2. Examples with separating variables

In this section, we study the spectral bands and dispersion relations in Cases A and B. To begin, we recall the spectral structure for the one-dimensional periodic problem.

2.1. The one-dimensional Sturm–Liouville problem. We consider the one-dimensional periodic spectral problem (Mathieu equation)

$$\widehat{H}_1\Phi = \mathcal{E}\Phi, \qquad \widehat{H}_1 = -\frac{h^2}{2}\frac{\partial^2}{\partial x^2} + v(x), \qquad v(x) = \frac{\omega_1^2}{2}(1-\cos x). \tag{5}$$

The spectrum of $\widehat{H}_1$ consists of those values $\mathcal{E}$ corresponding to nontrivial solutions Φ bounded in $\mathbb{R}$. It is known that the spectrum is positive and consists of bands $[\mathcal{E}_m^-, \mathcal{E}_m^+]$, $m = 0, 1, \ldots$, separated by gaps $(\mathcal{E}_m^+, \mathcal{E}_{m+1}^-)$ (see [2]). The eigenspace corresponding to each $\mathcal{E} \in [\mathcal{E}_m^-, \mathcal{E}_m^+]$ is spanned by Bloch solutions $\Phi^m(x,q)$, i.e., solutions with the property

$$\Phi^m(x+2\pi, q) = e^{2\pi i q}\Phi^m(x,q), \tag{6}$$

where $q \in [0,1)$ is called a quasimomentum. If $q = 0$ or $q = 1/2$, then the eigenspace is one-dimensional and spanned by a real-valued periodic function $\Phi^m(x,0)$ or antiperiodic function $\Phi^m(x,1/2)$. For any other q, the space is two-dimensional and spanned by $\Phi^m(x,q)$ and $\Phi^m(x,1-q) \equiv \overline{\Phi^m(x,q)}$.

All these properties hold without the assumption that the parameter h is small. We now study spectral bands as $h \to 0$ in detail. For a rough description of the bands and eigenfunctions, we can use the harmonic oscillator approximation near the point $x_k = 2\pi k$. The mth band is then located near the energy $\mathcal{E}_m(q) = h\omega_1(1/2+m) + O(h^2)$.

We construct functions $w_m(x) = \mathbf{H}_m(\omega_1 x/\sqrt{h})e^{-\omega_1 x^2/2h}$ and also $w_m^k(x) = C_m w_m(x - x_k)$, where $\mathbf{H}_m$ are Hermite polynomials and C_m are normalizing constants. Each function w_m^k is localized in a neighborhood of the point x_k. A rough approximation of the Bloch functions is given by

$$\widetilde{\Phi}^m(x,q) = \sum_{k=-\infty}^{\infty} w_m^k(x)e^{2\pi i k q}. \tag{7}$$

Each function $\widetilde{\Phi}^m(x,q)$ is thus localized in neighborhoods of the points x_k and defines the so-called power-law asymptotic approximation in h: the equality $(\widehat{H}_1 - \mathcal{E})\widetilde{\Phi}^m(x,q) = O(h^{3/2})$ holds.

Such an asymptotic approximation does not allow finding the exponentially small band width nor the dependence $\mathcal{E}_m(q)$. We should use a more precise WKB-type asymptotic approximation instead, where the functions w_m are replaced with

$$w_m(x) = A_m(x,h)e^{-\theta(x)/h}, \qquad \theta(x) = \left|\int_{x_k}^{x_k+x} \sqrt{2v(z)}\,dz\right|. \tag{8}$$

Therefore, $\theta(x)$ is in fact the value of the Maupertuis–Jacobi action calculated along the instanton (see Fig. 2). The amplitude $A_m(x,h)$ is a smooth function found from the transport equation and is close to $\mathbf{H}_m(\omega_1(x-x_k)/\sqrt{h})$ near x_k. We note that sum (7) is the known representation of Bloch functions in terms of Wannier functions and equality (8) determines the asymptotic approximation of the Wannier function.

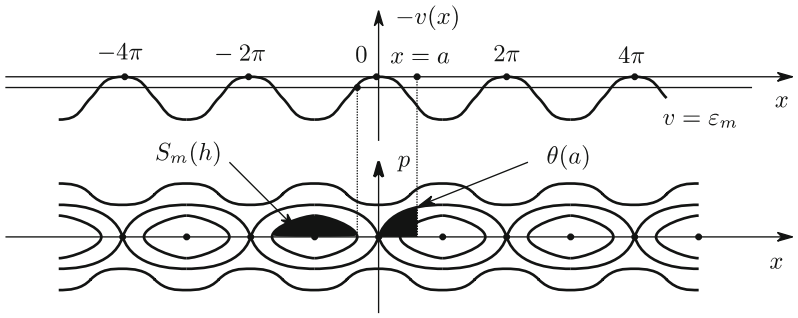


Fig. 2. (above) Graph of the inverted potential $-v(x)$ and (below) the phase portrait, i.e., level lines of the function $p^2/2 - v(x) = E$: the energy $E = 0$ corresponds to the instanton, and $E = -\mathcal{E}_m$ corresponds to the libration. The function $\theta(x)$ is the area under the graph of the instanton, and $S_m(h)$ is half the area of the domain surrounded by the libration $E = \mathcal{E}_m$.

It turns out that if the leading term of the function $A_m(x,h)$ and also the function $\theta(x)$ in asymptotic approximation (8) are known on the segment $[-\pi,\pi]$, then the band width and dispersion relations can be easily found. We discuss the calculations in more detail below and here only formulate the final result.

Let $S_m(h)$ be the Maupertuis–Jacobi action along the libration with the total energy $E = -\mathcal{E}_m$ (see Fig. 2), i.e.,

$$S_m(h) = \int_{x_-(h,m)}^{x_+(h,m)} \sqrt{2v(x) - h\omega_1(2m+1)}\,dx, \tag{9}$$

where $x_\pm(h,m)$ are points in the interval $x_k < x_-(h,m) < x_+(h,m) < x_{k+1}$ where the integrand in (9) vanishes.

Theorem 1. *The asymptotic formula*

$$\mathcal{E}_m(q) - \mathcal{E}_m(0) = (-1)^m b_m \frac{\omega_1 h}{\pi} e^{-S_m(h)/h}(1-\cos 2\pi q)(1+o(1)) \tag{10}$$

holds for the spectrum of operator (5)*, where b_m are constants independent of the potential* (*see* (17) *below*).

The dispersion relation curves on the plane (E,q) are shown in Fig. 3.

Remark 2. Formula (10) resembles the Landau–Lifshitz asymptotic formula for the widths of highly excited bands in a one-dimensional periodic problem (see Problem 3 in Sec. VI.55 in [6]). The dispersion relations for the lower bands "in terms of an instanton" are well known [14].

Remark 3. We derive formula (10) using the Herring method in Sec. 6 and present a rigorous proof by the Helffer–Sjöstrand method in Sec. 8. We also note that an advantage of the second approach is that it also works without requiring the symmetry $x \to -x$.

2.2. Cases A and B. *Case A.* It is easy to see that the spectrum of the operator $\widehat{H}$ can be represented in the form $E = E_{mn}(q) = \mathcal{E}_m(q) + \widetilde{\mathcal{E}}_n$, where $\widetilde{\mathcal{E}}_n = h\omega_2(n+1/2)$ and $\mathcal{E}_m(q)$ is the band spectrum of the one-dimensional periodic Sturm–Liouville operator. Here, $m = 0,1,\dots$ is the band number and q (mod 1) is a quasimomentum. The eigenfunctions Φ of $\widehat{H}$ are the products $\Phi^m(x,q)\widetilde{\Phi}^n(y)$ of the eigenfunctions $\widetilde{\Phi}^n(y)$ for the harmonic oscillator and the Bloch function $\Phi^m(x,q)$ (see the spectral structure in Fig. 4a).

Hence, the spectrum consists of bands. Under the additional nonresonance condition (i.e., ω_1 and ω_2 are rationally independent), the bands do not overlap for sufficiently small h.

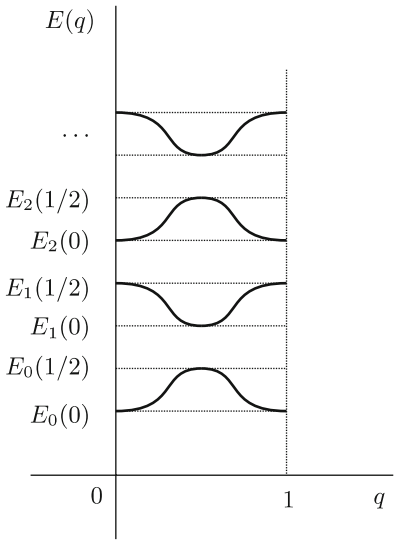


Fig. 3. Dispersion relations—quasimomenta and energy: the endpoints of bands correspond to periodic or antiperiodic Bloch functions.

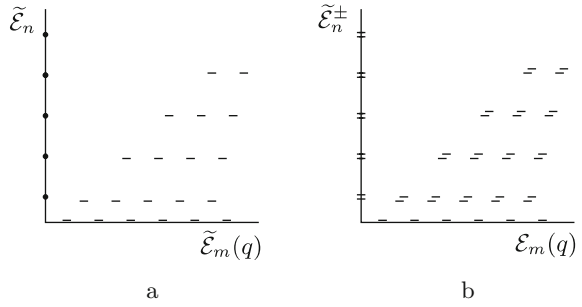


Fig. 4. The spectra in (a) Case A and (b) Case B: the spectral bands of the periodic operator are shown on the horizontal axis. The discrete spectrum of the harmonic oscillator in Case A and of the double-well potential $V(y)$ in Case B is shown on the vertical axis. In both cases, the segments are obtained by summing the eigenvalues on the axes. The spectrum of the two-dimensional operator is obtained by projecting these segments on the horizontal axis.

Case B. Let $V(y)$ be a symmetric double-well potential. The corresponding one-dimensional Schrödinger operator was studied in many works (see [3], [14]–[16]). Its spectrum is discrete, and eigenvalues near the potential minimums divide into asymptotically coinciding pairs $\widetilde{\mathcal{E}}_n^{\pm}$ as $h \to 0$. The leading term of their asymptotic expansion is determined by the harmonic oscillator approximation, and the difference between these values (splitting) is exponentially small:

$$\widetilde{\mathcal{E}}_n^{\pm} = \omega_2 h\left(n + \frac{1}{2}\right) + O(h^2), \qquad \widetilde{\mathcal{E}}_n^{+} - \widetilde{\mathcal{E}}_n^{-} = \widetilde{Q}_n(1 + o(1)), \quad h \to 0.$$

Remark 4. The leading term $\widetilde{Q}_n$ has a form similar to the right-hand side of (10) mutatis mutandis (see [15], [3]).

Hence, the spectrum in Case B has the form $E = E_{nm}(q) = \widetilde{\mathcal{E}}_n^{\pm} + \mathcal{E}_m(q)$. As in Case A, it consists of bands, which can now overlap (if the gap $\widetilde{\mathcal{E}}_n^{+} - \widetilde{\mathcal{E}}_n^{-}$ is sufficiently small compared with the band width $\mathcal{E}_m(1/2) - \mathcal{E}_m(0)$) (see the spectral structure in Fig. 4b).

As noted above, the spectral structure in Case 1 is close to Case A, and Case 2 resembles Case B. But we indicate one essential difference between Cases B and 2. Because of the richer symmetry in Case 2, there is an exact spectral degeneracy for some energy values. Namely, it turns out that the endpoints of bands corresponding to $q = 1/2$ coincide (exactly). This effect, generally speaking, does not occur in Case B, where we can find only conditions for "asymptotic," not exact, degeneracy.

3. Instantons and librations in two dimensions

Everywhere in this section, we work with the following classical system, which we naturally call the tunnel system. This is a Lagrangian system $L = T + U$ with the inverted potential $V = -U$ and the standard kinetic energy $T = (\dot{x}^2 + \dot{y}^2)/2$. The configuration space Z is a cylinder $x \pmod{2\pi/\beta}$, $y \in \mathbb{R}$. The system is equivalent to the Newtonian system $\ddot{x} = \partial U/\partial x$, $\ddot{y} = \partial U/\partial y$.

We fix a certain value of the energy E. Let V_E denote the domain of classically allowed motions with the energy E, i.e., $V_E = \{x \in Z\colon V(x) \le E\}$. In what follows, we are interested in special trajectories of the tunnel system reaching the boundary ∂V_E: (1) librations, i.e., periodic trajectories with the energy E reaching ∂V_E twice in a period and (2) instantons, i.e., doubly asymptotic (homoclinic or heteroclinic) trajectories connecting two unstable equilibriums associated with the maximum of V. (We recall that a solution is said to be homoclinic if it tends to a single point as $t \to \pm\infty$ and heteroclinic if it goes to two different points.)

At first glance, the question of the existence of instantons and librations resembles the known problem of closed geodesics on a Riemannian manifold. The question of the existence of such geodesics is resolved in the framework of Morse theory (see [17]), but those results are not directly applicable to the problem of finding librations (and also instantons), because librations reach the boundary of V_E, where the metric degenerates.

Theorem 2 [18], [19]**.** *Let M be compact and V_E not contain equilibriums. Let $V_E/\partial V_E$ be a quotient topological space (i.e., obtained from V_E by contracting ∂V_E to a point). Then the number of distinct librations is not less than the number of generators of the fundamental group $\pi(V_E/\partial V_E)$.*

Remark 5. The compactness assumption is formally violated in our case. Nevertheless, this difficulty can be easily overcome by perturbing the potential for large y and then compactifying the cylinder Z.

Remark 6. The existence of homoclinic and heteroclinic trajectories can be proved along the same lines. The difference is in the local analysis near the minimums of V (see [18], [19]).

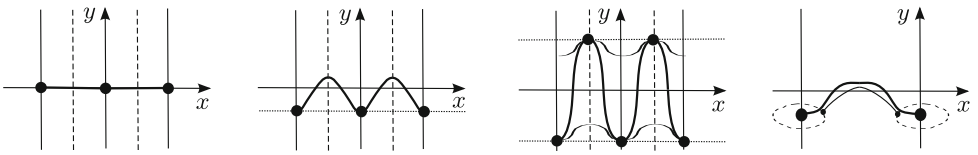
We recall that the Maupertuis–Jacobi action along a trajectory γ of a Lagrangian system $L = T + U$ with the energy $-E$ is defined as

$$d = \int_\gamma \sqrt{2(U(x) - E)}\, ds.$$

Here, $ds^2 = dx^2 + dy^2$ is the standard Euclidean metric. Below, the action is always the Maupertuis–Jacobi action. The metric $\sqrt{2(U(x) - E)}\, ds$ is called the Jacobi matric (or the Agmon metric in a semiclassical context).

The librations and instantons in Theorem 2 are the shortest paths between the corresponding connected components of ∂V_E in the Jacobi metric.

We return to the classical tunnel system. In Case 0, there is a unique well z_1, the system has an invariant plane $y = \dot{y} = 0$, and the instanton and librations are therefore solutions of the one-dimensional problem. In this simple case, we do not need Theorem 2. Clearly, the librations and the instanton project on the same line $y = 0$ in the configuration (physical) space (see Fig. 5a)).



a b c d

Fig. 5. Instantons in (a) Cases 0, (b) Case 1, and (c) Case 2: the horizontal axis is the x axis and the vertical axis is the y axis. The solid vertical lines are $x = 2\pi n/\beta$. The dashed vertical lines are the symmetry axes $x = (2n+1)\pi/\beta$, and the dashed horizontal lines are $y = \pm y_*$. (d) The instanton (bold) and the libration (thin): the dashed lines are two components of the potential energy level.

In Case 1, there is also a unique well z_1 on the cylinder Z. But things become more difficult compared with Case 0, and instantons and librations cannot be found analytically. The group $\pi(V_E/\partial V_E)$ is isomorphic to $\mathbb{Z}$ with a noncontractible closed cycle on the cylinder as generator. According to Theorem 2, this cycle determines an instanton (a homoclinic trajectory to z_1; see Fig. 5b)) and a family of librations encircling the cylinder.

The instantons and librations have the symmetry $x \to -x$. Consequently, they cross the symmetry line at a right angle. We also note that librations and instantons generally do not project on the same curve in the configuration space (see Fig. 5d)).

In Case 2, in addition to the axial symmetry $x \to -x$, the potential also has the central symmetry $y \to -y$, $x \to \pi/\beta - x$. As follows from Proposition 1, the potential has two wells z_1 and z_2, and the space $V_E/\partial V_E$ is homotopy equivalent to a cylinder with a handle (connecting z_1 and z_2). Then $\pi(V_E/\partial V_E)$ is the free group with two generators. According to Theorem 2, there exists a heteroclinic instanton, connecting z_1 and z_2. Because of the axial symmetry, we immediately obtain another instanton (they are shown by solid lines in Fig. 5c)). They correspond to two independent cycles on $V_E/\partial V_E$. The existence of other instantons generally cannot be guaranteed. Nevertheless, a noncontractible instanton homoclinic to z_1 can exist under the condition that the wells z_1 and z_2 are located sufficiently far apart. (More precisely, the distance between them in the Jacobi metric should be greater than the distance between the two nearest preimages of z_1 on the covering space $\mathbb{R}^2$.) This can happen when β is large. A numerical analysis indicates that there is no homoclinic instanton for $\beta = 1$ (the interesting case for application to dimers). The homoclinic instantons are shown by dashed lines in Fig. 5c.

Hence, heteroclinic instantons have the central symmetry (in particular, they cross the x axis at $x = \pm\pi(2n+1)/2\beta$), and homoclinic instantons have the axial symmetry. Moreover, the axial symmetry converts a heteroclinic instanton into another heteroclinic instanton, and the central symmetry converts a homoclinic instanton into another homoclinic instanton.

4. Main results

We study the spectral bands of operator (1). For convenience, we pass from the potential U to $U - U_{\min}$ with the global minimum is $U = 0$. This new potential is also denoted by U. We recall that the harmonic oscillations frequencies are denoted by $\omega_{1,2}$; they can be easily calculated:

$$\omega_1 = \sqrt{\beta r}, \qquad \omega_2 = \sqrt{1+r}, \quad \text{where } r = \alpha|\cos(y_* - y_0)|.$$

(Hence, ω_1 corresponds to the x axis and ω_2 corresponds to the y axis.) Let ω_- denote the least frequency and ω_+ denote the greatest frequency.

In what follows, we assume that the following *nondegeneracy conditions* are satisfied:

1. The frequencies ω_1 and ω_2 are rationally independent.
2. We have $\omega_+ > 2\omega_-$.
3. There is a unique instanton on the cylinder Z in Case 1 and at most two homoclinic and two heteroclinic instantons on Z in Case 2.
4. Each instanton approaches each equilibrium z_k in a nonsingular direction, i.e., the direction of the axis corresponding to ω_-.
5. The asymptotic manifolds of the unstable equilibriums z_k intersect transversely along each instanton.

We discuss sufficient conditions for some of these conditions to be satisfied in the physically interesting case $\beta = 1$.

Proposition 2. *Let $\beta = 1$, $r \le 1/3$, and $r \ne q_1^2/(q_1^2 - q_2^2)$ for $q_1, q_2 \in \mathbb{Z}$. Then $\omega_- = \omega_1$, and conditions* 1, 2, *and* 4 *are satisfied.*

Proof. Conditions 1 and 2 can be easily verified. To prove that condition 4 is satisfied, we note that only two asymptotic solutions approach the unstable equilibrium in the singular direction, which corresponds to ω_2 according to the assumptions. (Indeed, the equilibrium has a node singularity on the two-dimensional stable asymptotic manifold.) From the tunnel system equations, we can see that the x coordinate is constant along those asymptotic solutions. Hence, those solution are not instantons. ■

Remark 7. Condition 2 is technical and can apparently be dropped. If so, then the assumption $r \le 1/3$ is also inessential.

Remark 8. Conditions 3 and 5 are generically satisfied, but checking them in a concrete situation is nontrivial. We do not discuss this problem here.

We introduce some important constructions, which are needed for describing the spectrum.

According to condition 3, the tunnel system $L = T + U$ has an instanton γ with zero total energy, $E = T - U = 0$. There is a family of librations γ_ε with energies $T - U = -\varepsilon < 0$ in a vicinity of this instanton. Let $\lambda(\varepsilon) > 0$ be a nontrivial Floquet exponent of a corresponding libration. It is easy to see that the equation

$$\varepsilon + \frac{h}{2}\lambda(\varepsilon) = \frac{h}{2}(\omega_-(2m+1) + \omega_+) \tag{11}$$

has a unique solution $\varepsilon = \varepsilon_m(h)$ for each $m = 0, 1, 2, \ldots$ and sufficiently small h and ε. This determines a sequence of energies $\varepsilon = \varepsilon_m(h)$ or a sequence of librations $\gamma_{\varepsilon_m(h)}$. We call them tunnel librations.

Remark 9. It is clear that librations in the one-dimensional case are just periodic orbits with energies of lower quantum states taken with the minus sign.

We note that the problem of seeking the Bloch functions with $q = 0$ (i.e., $2\pi/\beta$-periodic in x) is equivalent to the problem of seeking the eigenfunctions of the Schrödinger operator on the cylinder Z. Further, to seek the Bloch functions with $q = 1/2$ (i.e., $2\pi/\beta$-antiperiodic in x), we can study the operator on the "twofold cylinder": $Z_{(2)} = \{x \pmod{4\pi/\beta},\, y \in \mathbb{R}\}$. Its eigenfunctions correspond not only to antiperiodic but also to periodic Bloch functions. More generally, the study of Bloch functions with rational quasimomenta leads to the operator on the "N-fold cylinder": $Z_{(N)} = \{x \pmod{2N\pi/\beta},\, y \in \mathbb{R}\}$. In what follows, all mathematically rigorous theorems about the spectrum are stated only for the case of rational quasimomenta.

Theorem 3. *We suppose that conditions* 1–5 *are satisfied and that we have Case* 1. *Then the set of points* $E \in [0, Ch]$ *such that there is a rational* $q \in [0, 1)$ *and a function* $\psi \in L^2(Z_{(N)})$ *satisfying the property*

$$\widehat{H}\psi = E\psi, \qquad \psi\left(x + \frac{2\pi}{\beta}, y\right) = e^{2\pi i q}\psi(x, y), \tag{12}$$

consists of elements $E = E_\nu(q)$, *where* $\nu = (\nu_-, \nu_+) \in \mathbb{Z}_+^2$ *such that the asymptotic approximation*

$$E_\nu(q) = \omega_-\left(\nu_- + \frac{1}{2}\right)h + \omega_+\left(\nu_+ + \frac{1}{2}\right)h + O(h^2) \tag{13}$$

holds. Furthermore,

a. *one and only one function (up to a constant factor) that satisfies* (12) *for a given* q *corresponds to each* $E = E_\nu(q)$,

b. $E_\nu(q) = E_\nu(1 - q)$,

c. *the dispersion relations*

$$E_\nu(q) - E_\nu(0) = 2\mathcal{A}(h)(\cos 2\pi q - 1)(1 + o(1)) \tag{14}$$

hold,

d. *there are constants* $\kappa_k = \kappa_k(\nu)$ *and* $C_1, C_2 > 0$ *such that*

$$C_1 h^{\kappa_1} e^{-d_0/h} \le |\mathcal{A}(h)| \le C_2 h^{\kappa_2} e^{-d_0/h}, \tag{15}$$

where d_0 *is the action along the instanton (unique up to the symmetry), and*

e. *if* $\nu_+ = 0$, *then*

$$|\mathcal{A}(h)| = b_{\nu_-}\frac{\omega_- h}{\pi}e^{-S(\varepsilon_{\nu_-}(h))/h}(1 + o(1)), \quad h \to 0, \tag{16}$$

where $S(\varepsilon_m(h))$ *is the action along half the period of the tunnel libration* $\gamma_{\varepsilon_m(h)}$ *and*

$$b_m = \frac{2^{-m}\sqrt{\pi}(2m + 1)^{(2m+1)/2}}{m! e^{m+1/2}}. \tag{17}$$

Comment 1. Therefore, the spectrum in Case 1 has a band structure: each quantum vector $\nu \in \mathbb{Z}_+^2$ is associated with a band located according to harmonic oscillator approximation (13). The dispersion relations are (14). The band width has upper and lower bounds (15) written in terms of the instanton action. For special quantum vectors, namely, such that $\nu_+ = 0$, the band width has an asymptotic approximation written in terms of the action along tunnel libration (16).

We proceed to Case 2. Let d_{het} be the action along the heteroclinic instanton and d_{hom} be the action along the homoclinic instanton. If the latter does not exist, then we formally set $d_{\text{hom}} = \infty$. Below, we consider two general situations: $d_{\text{het}} < d_{\text{hom}}$ and $d_{\text{hom}} < d_{\text{het}}$.

Theorem 4. *We suppose that conditions* 1–5 *are satisfied and that we have Case* 2. *Moreover, let* $d_{\text{het}} < d_{\text{hom}}$ (*including the case* $d_{\text{hom}} = \infty$). *Then the set of points* $E \in [0, Ch]$ *such that there is a rational* $q \in [0, 1)$ *and a function* $\psi \in L^2(Z_{(N)})$ *satisfying property* (12) *consists of elements* $E = E_\nu^+(q)$ *and* $E = E_\nu^-(q)$, *where* $\nu = (\nu_-, \nu_+) \in \mathbb{Z}_+^2$ *such that asymptotic approximation* (13) *holds. Furthermore,*

a.1. *if* $q \neq 1/2$, *then one and only one function* (*up to a constant factor*) *that satisfies* (12) *for a given* q *corresponds to each* $E = E_\nu^\pm(q)$,

a.2. $E_\nu^+(1/2) = E_\nu^-(1/2)$, *this value is associated with a two-dimensional space of functions satisfying* (12) *for* $q = 1/2$,

b. $E_\nu(q) = E_\nu(1-q)$,

c. *the dispersion relations*

$$E_\nu^\pm(q) - E_\nu^\pm\left(\frac{1}{2}\right) = \pm\mathcal{A}(h)(1+\cos 2\pi q)(1+o(1)), \quad h \to 0, \tag{18}$$

hold,

d. *estimates* (15) *are applicable, where* $d_0 = d_{\rm het}$,

e. *if* $\nu_+ = 0$, *then asymptotic approximation* (16) *holds, and librations are chosen near the heteroclinic instanton.*

Comment 2. Therefore, in Case 2 for $d_{\rm het} < d_{\rm hom}$, each quantum vector $\nu \in \mathbb{Z}_+^2$ is associated with a pair of bands $I_\nu^\pm = \bigcup_{q\in[0,1)} E_\nu^\pm(q)$ located, as before, according to the harmonic oscillator approximation. These bands are adjacent at their endpoints corresponding to $q = 1/2$, where there is an exact degeneracy. The dispersion relations and both band widths are found by formulas similar to those in Case 1. The dispersion relations presented in Theorem 4 define curves on the plane (E, q) shown in Fig. 6a.

Theorem 5. *We suppose that conditions* 1–5 *are satisfied and that we have Case 2. Moreover, let* $d_{\rm hom} < d_{\rm het}$. *Then the set of points* $E \in [0, Ch]$ *such that there is a rational* $q \in [0,1)$ *and a function* $\psi \in L^2(Z_{(N)})$ *satisfying property* (12) *consists of elements* $E = E_\nu^+(q)$ *and* $E = E_\nu^-(q)$, *where* $\nu = (\nu_-, \nu_+) \in \mathbb{Z}_+^2$, *such that asymptotic approximation* (13) *holds. Furthermore,*

a.1. *if* $q \neq 1/2$, *then there is at most a two-dimensional space of functions that satisfy* (12) *for a given* q *and* $E = E_\nu^\pm(q)$ *corresponds to each pair* (ν, q),

a.2. $E_\nu^+(1/2) = E_\nu^-(1/2)$, *which value is associated with a two-dimensional space of functions satisfying* (12) *for* $q = 1/2$,

b. $E_\nu(q) = E_\nu(1-q)$,

c. *the dispersion relations*

$$E_\nu^\pm(q) - E_\nu^\pm\left(\frac{1}{2}\right) = 2\mathcal{A}(h)(1+\cos 2\pi q)(1+o(1)), \quad h \to 0, \tag{19}$$

hold,

d. *estimates* (15) *are applicable, where* $d_0 = d_{\rm hom}$,

e. *if* $\nu_+ = 0$, *then asymptotic approximation* (16) *holds, and librations are chosen near the homoclinic instanton.*

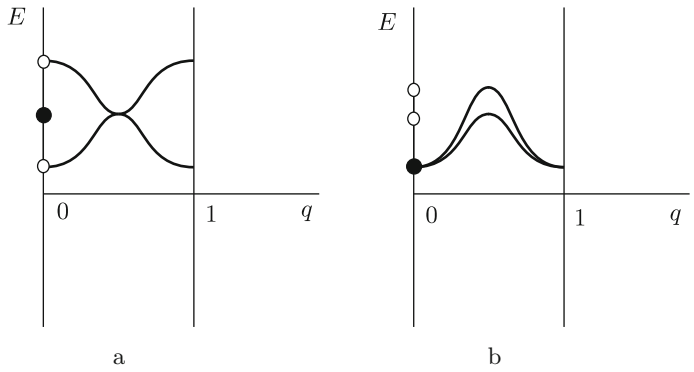


Fig. 6. Dispersion relations in Case 2: (a) $d_{\mathrm{het}} < d_{\mathrm{hom}}$ and (b) $d_{\mathrm{hom}} < d_{\mathrm{het}}$.

Comment 3. Therefore, in Case 2 for $d_{\mathrm{hom}} < d_{\mathrm{het}}$, each quantum vector $\nu \in \mathbb{Z}^2_+$ is associated with a pair of overlapping bands $I^{\pm}_{\nu} = \bigcup_{q\in[0,1)} E^{\pm}_{\nu}(q)$ located, as before, according to the harmonic oscillator approximation. Exact degeneracy occurs at the endpoints corresponding to $q = 1/2$. The dispersion relations and band widths are calculated by similar formulas. These bands virtually coincide, and it can even happen that the exact degeneracy holds for all q, not only for $q = 1/2$, which is why the theorem states that the pair E and q may correspond to a two-dimensional space of Bloch functions. If there is no degeneracy, then as in Theorem 4, each E and $q \neq 1/2$ corresponds to a unique Bloch function. We note that such effects are very subtle, and we do not know satisfactory methods for treating them. The dispersion relations in Theorem 5 define a curve on the plane (E, q) shown in Fig. 6b.

Remark 10. A numerical analysis allows claiming that for $\beta = 1$ (i.e., in the case of dimers) in Case 2, the conditions in Theorem 4 are satisfied, and there are no homoclinic instantons.

5. Numerical calculations

Asymptotic formula (16) has the advantage that almost all its components can be quite easily found numerically with any given precision. The main difficulty is to find a tunnel libration.

5.1. Seeking the tunnel libration. A libration with a given energy $-E < 0$ can be found numerically relatively easily thanks to the symmetry and also because of the small dimension. The method slightly differs for Case 1 and Case 2. We set $\beta = 1$ for simplicity.

In Case 1 (see Fig. 7a), we assume that y_0 is chosen such that the wells are located on the lines $x = 2\pi n$. We solve a Cauchy problem with the initial conditions

$$x(0) = \pi, \qquad y(0) = a, \qquad p_x(0) = \sqrt{2(U(\pi, a) - E)}, \qquad p_y = 0.$$

The parameter a can vary. A libration is defined by $a = a_0$ if the trajectory returns to the line $x_0 = \pi$ and intersects it at $y = a_0$. In a small neighborhood of a_0, we can construct a map $A = \mathcal{P}(a)$, where $y = A$ is the y coordinate of the next intersection with the line $x = \pi$. Clearly, $\mathcal{P}(a_0) = a_0$.

To find a libration numerically, we start from a small segment $[a_1, a_2]$ such that $\mathcal{P}(a_1) > a_1$ and $\mathcal{P}(a_2) < a_2$ and use bisections until we reach the needed accuracy.

In Case 2 (see Fig. 7b), the same method can be used to find a "horizontal" libration (the one close to a homoclinic instanton). To find a "vertical" libration (the one close to a heteroclinic instanton), we choose initial conditions as

$$x(0) = \frac{\pi}{2}, \qquad y(0) = 0, \qquad p_x = r\cos a, \qquad p_y = r\sin a,$$

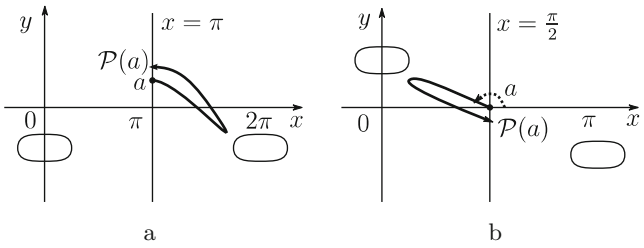


Fig. 7. Seeking a libration numerically: (a) In Case 1, we shoot from the line $x = \pi$ with the initial velocity parallel to the x axis, the magnitude of the velocity is determined by the energy E, and the varied parameter a is the initial y coordinate. (b) In Case 2 for a "vertical" libration, we shoot from the point $x = \pi/2$, $y = 0$, the velocity magnitude is determined by the energy E, and the varied parameter a is the shooting angle.

where $r = \sqrt{2(U(\pi/2, 0) - E)}$. The varied parameter a is now the shooting angle. As before, we define a map $Y = \mathcal{P}(a)$, where $y = Y$ is the y coordinate of the next intersection of the trajectory with the line $x = \pi/2$. The libration corresponds to a solution of $\mathcal{P}(a_0) = 0$. Again, we start from a small segment $[a_1, a_2] \ni a_0$ and then use the bisection method.

We note that the map $\mathcal{P}$ is sensitive to small changes of the argument in both cases because librations are unstable trajectories. For instance, a segment $[a_1, a_2]$ that contains a libration should have length of order 10^{-2} or 10^{-3}.

We rewrite Eq. (11) as

$$\varepsilon = f(\varepsilon), \qquad f(\varepsilon) = \frac{h\omega_1}{2} + \frac{h(\omega_2 - \lambda(\varepsilon))}{2}.$$

Its solution yields a tunnel libration. We seek it by the iterative process:

$$\varepsilon_0 = \frac{h\omega_1}{2}, \qquad \varepsilon_n = f(\varepsilon_{n-1}).$$

On each step, we need to find a libration with given energy and also calculate its positive Floquet exponent. Concrete calculations (see below) indicate that the iteration process converges rapidly. The first iteration already gives sufficiently high accuracy.

5.2. Numerical results. To illustrate our method, we take $\alpha = 1$, $y_0 = \pi/2$ (Case 2), and different $h \in [0.05, 0.09]$. Therefore, the parameter h is neither too small nor too large. Given this choice, the semiclassical approximation is applicable, and the tunnel effects are still perceptible.

In this example, $E_{\min} = -0.400488$ is the minimum energy value, $\omega_1 = 0.859700$, and $\omega_2 = 1.318743$. The band widths ΔE_0, ΔE_1, and ΔE_2 are calculated using the asymptotic formulas mentioned above with the quantum vectors $\nu_k = (k, 0)$, $k = 0, 1, 2$ (we recall that the first component corresponds to the direction of the instanton). The positions of these bands are shown on Fig. 8. Some of the bands cannot be thought of as "low." Nevertheless, the right-hand side of (16) can be numerically calculated, although it may differ drastically from the left-hand side, as we leave the neighborhood of the bottom of the well.

In Tables 1, 2, and 3 (corresponding to $\nu = \nu_0, \nu_1, \nu_2$), we show the energies of librations during the iterative process described above. We stress that the procedure converges rapidly even in the case where the state is quite far from the bottom of the well.

Once a tunnel libration has been found, we can easily compute the band widths (see Fig. 9, where we present the final numerical results).

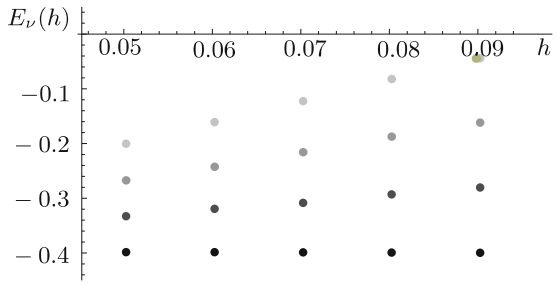


Fig. 8. Energy levels $E_\nu(h)$: the lowest value is $E_{\min}$, then $E_\nu(h)$ for $\nu = \nu_0, \nu_1, \nu_2$, the value $E = 0$ is the next critical point of $U(x, y)$.

Table 1

Iteration	$h = 0.05$	$h = 0.06$	$h = 0.07$	$h = 0.08$	$h = 0.09$
0	−0.378996	−0.374698	−0.370399	−0.366101	−0.361802
1	−0.377707	−0.373156	−0.368607	−0.36406	−0.359514
2	−0.377709	−0.373158	−0.36861	−0.364063	−0.359519

Table 2

Iteration	$h = 0.05$	$h = 0.06$	$h = 0.07$	$h = 0.08$	$h = 0.09$
0	−0.336011	−0.323116	−0.31022	−0.297325	−0.284429
1	−0.334764	−0.32163	−0.308499	−0.29537	−0.282242
2	−0.334765	−0.321632	−0.308501	−0.295372	−0.282244

Table 3

Iteration	$h = 0.05$	$h = 0.06$	$h = 0.07$	$h = 0.08$	$h = 0.09$
0	−0.293026	−0.271534	−0.250041	−0.228548	−0.207056
1	−0.291807	−0.270083	−0.24836	−0.226639	−0.204918
2	−0.291807	−0.270083	−0.248361	−0.22664	−0.204919

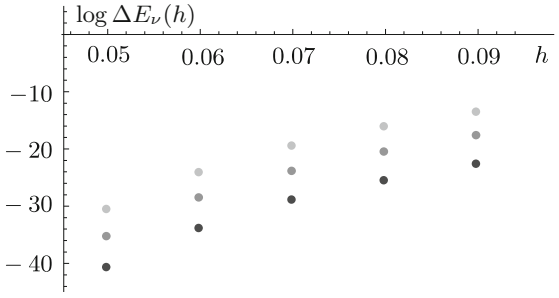


Fig. 9. Band widths on a logarithmic scale.

Concluding this section, we emphasize that this algorithm works well for arbitrarily small h, although a greater accuracy of numerical integration may be required.

6. Spectral bands, Wannier functions, and their asymptotic approximations

In this section, we give a "hand-waving" explanation of some of our results presented in Sec. 4. We do not add mathematically rigorous meaning to this argument, because rigorous proofs by another method follow below. For simplicity, we restrict ourself to a one-dimensional case (Theorem 1), but the arguments can be easily extended to Case 1.

We recall a useful formula relating Bloch function $\Phi^m(x,q)$ to the Wannier functions (see [6]). Because the functions $\Phi^m(x,q)$ are one-periodic in q, they can be expanded in Fourier series:

$$\Phi^m(x,q) = \sum_{l\in\mathbb{Z}} c_l(x) e^{2\pi i q l}, \tag{20}$$

where it follows from Bloch condition (6) that $c_l(x) = c_0(x - 2\pi l)$. The function c_0 is called a Wannier function and is denoted by $\zeta^m(x)$. Hence,

$$\Phi^m(x,q) = \sum_{l=-\infty}^{\infty} \zeta^m(x - 2\pi l, y) e^{2\pi i q l}. \tag{21}$$

Proposition 3. *The Wannier functions $\zeta^m(x)$*

1. *are even,*

2. *decay exponentially as $x \to \infty$, and*

3. *are quasimodes, i.e., functions satisfying the Schrödinger equation up to an error exponentially small in h.*

Corollary 1. *The Wannier functions ζ^m admit a WKB-type approximation $\zeta^m = (A+O(h))e^{-S(x)/h}$.*

Remark 11. This approximation is close to the Gaussian exponential function ($S = \alpha x^2/2$) in a neighborhood of a minimum of the potential $v(x)$.

The idea of the proof of Proposition 3 is presented in Appendix B.

We define a normalized Wannier function $\zeta_0^m = \zeta^m/\|\zeta^m\|$. The following result is a version of the Landau–Lifshitz formula (see [5]).

Proposition 4. *The dispersion relation for the mth band of one-dimensional operator* (5) (*for all $0 < q < 1$*) *is*

$$E_m(q) - E_m(0) = -2h^2 \zeta_0^m(\pi)\zeta_0^{m\prime}(\pi)(1 - \cos 2\pi q)(1 + o(1)). \tag{22}$$

The idea of the proof Proposition 4 is presented in Appendix C.

To derive Theorem 1 from Proposition 4, we should evaluate $\zeta_0^m(\pi)$ and $(\zeta_0^m)'(\pi)$ from the Hamilton–Jacobi and transport equations with sufficient accuracy. We postpone the details of this argument until Sec. 8.

7. Interaction matrix

In this section, we recall the main facts from the Helffer–Sjöstrand theory, presented in [3], about the semiclassical asymptotic approximation of a Schrödinger operator with a potential with a finite number of wells. The operator acts in $L^2(M)$, where for our purposes we can take a cylinder or a circle as the manifold M, i.e.,

$$M = \left\{ x \left(\operatorname{mod} \frac{2\pi N}{\beta} \right),\ y \in \mathbb{R}^{n-1} \right\}, \quad n = 1, 2.$$

We assume that the potential $\widetilde{U}$ is a smooth function such that $\widetilde{U} \to \infty$ as $y \to \infty$. We do not yet impose any symmetry assumption. Let $z_1, \dots, z_m \in M$ be global minimums (wells) of $\widetilde{U}$, and let them be nonresonant, i.e., for all $1 \le l \le m$,

$$\sum_{j=1}^{n} k_j \omega_{l,j} \neq 0 \quad \text{for all } 0 \neq k \in \mathbb{Z}^n,$$

where $\omega_{l,j}$ are harmonic oscillator frequencies associated with the lth well.

It is well known that up to $O(h^\infty)$, the spectrum (more precisely, its lower part) of $\widehat{H}$ is just the union of the spectra Spec_l, $l = 1, \dots, m$, associated with each well. Namely, we take any small neighborhood Ω_l of some well z_l and then multiply $\widetilde{U}$ by a cutoff function with support in Ω_l. Then Spec_l is simply the spectrum of the Schrödinger operator with Dirichlet boundary conditions on $\partial\Omega_l$.

Principle terms of eigenvalues in Spec_l are determined from the harmonic oscillator approximation:

$$\operatorname{Spec}_l = \left\{ \sum_{j=1}^{n} \frac{\omega_{l,j} h}{2} (2\nu_j + 1) + O(h^2),\ \nu = (\nu_1, \dots, \nu_n) \in \mathbb{Z}_+^n \right\}.$$

We note that all principle terms in Spec_l are distinct because of the nonresonance assumption.

We assume that the lower parts of Spec_l coincide up to $O(h^\infty)$ (e.g., because of a symmetry, but not necessarily). The spectrum of $\widehat{H}$ is then m-fold nearly degenerate (up to $O(h^\infty)$).

We fix $\nu \in \mathbb{Z}_+^n$ and define I as a small ($\sim h^2$) interval containing exactly one eigenvalue of each Spec_l associated with ν.

We let $d_E(u, v)$ denote the distance between u and v on M in the Jacobi metric $\sqrt{2(\widetilde{U}(x, y) - E)}\, ds$. We define the distance between wells as $\sigma_0 = \min_{j \neq k} d_0(z_j, z_k)$. We choose a small $\delta > 0$ and an arbitrary $\sigma \in (0, \sigma_0 - \delta)$.

We let $B(z, r) \subset M$ denote a ball of radius r in the sense of the Jacobi distance d_0 with the center z. We set $B_k = B(z_k, \delta)$ and $M_j = M \setminus \bigcup_{k \neq j} B_k$ and let $\widehat{H}_j$ be a self-adjoint extension of $\widehat{H}$ on $L^2(M_j)$ with Dirichlet boundary conditions. The spectrum $\operatorname{Spec} \widehat{H}_j$ is nondegenerate, and $I \cap \operatorname{Spec} \widehat{H}_j$ contains a single element $\mathcal{E}_j$. Let ψ_j be the associated normalized eigenfunctions.

Theorem 6 [3]**.** 1. *Under the above assumptions, $I \cap \operatorname{Spec} \widehat{H}$ contains exactly m eigenvalues (counting multiplicities).*

2. *The matrix P of the operator $\widehat{H}|_{\mathcal{V}_\nu}$, where $\mathcal{V}_\nu$ is the span of the eigenfunctions from point* 1*, in some orthonormal basis has the form*

$$P = \operatorname{diag}(\mathcal{E}_1, \dots, \mathcal{E}_m) + W + O(e^{-2\sigma/h}),$$

where the matrix $W = (w_{jk})$ has the elements

$$w_{jk} = \frac{h^2}{2} \int_{\partial\Omega_{jk}} \left(\psi_j \frac{\partial \psi_k}{\partial n} - \psi_k \frac{\partial \psi_j}{\partial n} \right) dS + O(e^{-2\sigma/h}), \tag{23}$$

$\Omega_{jk} \subset M$ *is a domain such that*

$$z_j \in \Omega_{jk}, \qquad z_k \notin \Omega_{jk}, \qquad \partial\Omega_{jk} \subset M_j \cap M_k,$$

and n *is the outward normal to the surface* $\partial\Omega_{jk}$.

The matrix P is called an interaction matrix.

Remark 12. The basis in Theorem 6 is close to a nearly orthonormal system $\psi_1, \dots, \psi_n$.

Remark 13. It can be shown that $w_{jk} = w_{kj}$.

For practical calculations, we can replace ψ_j in (23) with their tunnel WKB approximations

$$\widetilde{\psi}_j(z) = \sum_{l=0}^{\infty} A_l^j(z) e^{-S_j(z)/h},$$

where the phase S_j is just the Agmon distance, $S_j(z) = d_0(z_j, z)$, and A_l^j are found from standard transport equations. Although $\widetilde{\psi}_j$ are only quasimodes (i.e., they satisfy the stationary Schrödinger equation with small discrepancy), it was shown in [3] that they are very close to the actual eigenfunctions ψ_j. As a result, the statement of Theorem 6 still holds if the eigenfunctions are replaced with the quasimodes.

8. Proofs of main theorems

We start by proving Theorem 1 for $m = 0$ and $q = 1/2$ using the approach in Sec. 7. It is inessential in our argument that the potential has form (5). It suffices to assume that $v(x)$ is a smooth periodic function with a unique point of global maximum. We again stress that the symmetry $x \to -x$ is not required. We study the case of arbitrary q later (see more details in Appendix D).

We now proceed to prove the theorems in Sec. 4. For simplicity, we assume that $\beta = 1$ without loss of generality.

Proof of Theorem 3. We first establish the estimates and asymptotic approximations for the band widths (i.e., dwell on the case $q = 1/2$). For this, we consider the operator $\widehat{H}$ on the cylinder $Z_{(2)}$. According to Theorem 6, the operator $\widehat{H}|_{\mathcal{V}_\nu}$ is determined by the matrix

$$P = \mathcal{E}I + W + O(e^{-2\sigma/h}) \equiv \begin{pmatrix} \mathcal{E} & w_{12} \\ w_{12} & \mathcal{E} \end{pmatrix} + O(e^{-2\sigma/h}).$$

The eigenvalues and eigenvectors of the matrix $\mathcal{E}I + W$ are

$$v_1 = (1,1), \quad v_2 = (1,-1), \qquad \lambda_1 = \mathcal{E} - w_{12}, \quad \lambda_2 = \mathcal{E} + w_{12}.$$

Hence, the space $\mathcal{V} = \mathcal{V}_\nu$ can be decomposed into a direct sum of the one-dimensional invariant subspaces $\mathcal{V}^{(1)}$ and $\mathcal{V}^{(2)}$ corresponding to λ_1 and λ_2.

We introduce the symmetry operator $G\psi(x,y) = \psi(x + 2\pi, y)$. Clearly, its eigenvalues are $\{\pm 1\}$. Because $\widehat{H}$ commutes with G, the spaces $\mathcal{V}^{(1)}$ and $\mathcal{V}^{(2)}$ are invariant under G. Therefore, $\mathcal{V}^{(1)}$ and $\mathcal{V}^{(2)}$ are spanned by 4π-periodic functions. From the form of the eigenvectors of $\mathcal{E}I + W$, using Remark 12, we easily see that $\mathcal{V}^{(1)}$ consists of 2π-periodic functions and $\mathcal{V}^{(2)}$ consists of 2π-antiperiodic functions.

We have thus found two points of the spectrum that correspond to Bloch functions with $q = 0$ and $q = 1/2$. The band width is then just the difference between the eigenvalues of P, i.e., it has the asymptotic approximation $2w_{12}$. Using the symmetry $x \to -x$, we obtain

$$E_\nu\left(\frac{1}{2}\right) - E_\nu(0) = 2w_{12}(1 + o(1)) = h^2(1 + o(1)) \int_\Sigma \left(\psi_1 \frac{\partial \psi_2}{\partial x} - \psi_2 \frac{\partial \psi_1}{\partial x}\right) dy, \quad h \to 0,$$

where Σ is a small segment of the line $x = \pi$ containing the intersection with the instanton. It is easy to see that we obtain the same expression that arises in the double-well problem. It is now possible to use known estimates [7] to obtain point d and asymptotic approximations (see [10], [11], [20]) to prove point e. Namely, Case 0 with $m = 0$ was considered in [10], and Case 1 was considered later in [11]. A generalization to arbitrary m was obtained in [20].

We now derive the dispersion relations. We take $q = l/N$ for $N = 2n$ and the cylinder $Z_{(N)}$. The potential then has N wells, and $W = w_{12}\Omega_N$, where

$$\Omega_N = (\omega_{jk}) \in \mathbb{R}^{N^2} \colon \omega_{jk} = 0, \qquad \text{except } \omega_{j,\,j+1} = \omega_{j+1,\,j} = 1, \tag{24}$$

where $1 \le j \le N$ and the indices are understood modulo N. The eigenvectors and eigenvalues of this matrix are

$$v_k = (1, e^{\pi i k/n}, e^{2\pi i k/n}, \dots, e^{\pi i k(2n-1)/n}), \qquad \lambda_k = 2w_{1\,2} \cos\frac{\pi k}{n}, \tag{25}$$

where $k = 0, \dots, 2n-1$. Therefore, the space $\mathcal{V} = \mathcal{V}_\nu$ can be decomposed into a direct sum of the invariant subspaces $\mathcal{V}^{(0)}, \dots, \mathcal{V}^{(n)}$ corresponding to λ_k and λ_{2n-k}, and

$$\dim \mathcal{V}^{(0)} = \dim \mathcal{V}^{(n)} = 1, \qquad \dim \mathcal{V}^{(k)} = 2, \quad 1 < k < n.$$

We introduce a symmetry operator acting by the same rule as before, $G\psi(x, y) = \psi(x + 2\pi, y)$, but now in the space $L^2(Z_{(N)})$. Clearly, its eigenvalues are the $2n$th roots of unity. Because $\widehat{H}$ commutes with G, the spaces $\mathcal{V}^{(k)}$ are invariant with respect to G. Hence, $\mathcal{V}^{(0)}$ and $\mathcal{V}^{(n)}$ are generated by a Bloch eigenfunction with $q = k/2n$. Because

$$v_0 = (1, 1, \dots, 1), \qquad v_n = (1, -1, \dots, 1, -1),$$

using Remark 12, we easily see that $\mathcal{V}^{(0)}$ is generated by a Bloch function with $q = 0$ and $\mathcal{V}^{(n)}$ by a Bloch function with $q = 1/2$.

We note that the eigenvalues of $G|_{\mathcal{V}^{(k)}}$ for $1 \le k < n$ are neither 1 nor -1. Indeed, the subspace of $\mathcal{V}$ generated by Bloch eigenfunctions with $q = 0, 1/2$ is two-dimensional (this is easily seen by considering the operator on the cylinder $Z_{(2)}$ with two wells). Therefore, the eigenvalues of $G|_{\mathcal{V}^{(k)}}$ are a complex conjugate pair of $2n$th roots of unity. It follows from (25) and also Remark 12 that $\mathcal{V}^{(k)}$ are generated by a pair of Bloch eigenfunctions with $q = k/2n, (2n-k)/2n$ and the associated eigenvalue has the multiplicity 2.

We have thus established the dispersion relations for all $q \in \mathbb{Q}$, and Theorem 3 is proved. ■

Remark 14. It is clear that the same dispersion relation (14) is satisfied in the one-dimensional case. The value $w_{1\,2}$ can be calculated as in Appendix D, and we obtain the right-hand side of (35), divided by two for $n \ge 2$. The latter follows because the instanton intersects the set $\partial\Omega_{1\,2}$ at a single point, not at two points. This implies Theorem 1 for $m = 0$ and any rational q.

The proofs of Theorems 4 and 5 are presented in Appendix E.

Appendix A: Proof of Proposition 1

We first note that the global minimum of the potential is negative: $U_{\min} < 0$. Indeed,

$$\min\left\{U(0,0), U\left(\frac{\pi}{\beta}, 0\right)\right\} \le -\alpha|\cos y_0|.$$

Therefore, $U_{\min} < 0$ in Case 1. In Case 2, $U(0,y)$ has a first degree of smallness in $y = 0$, and therefore again $U_{\min} < 0$.

The critical points of $U(x,y)$ are found from the equations

$$y + \alpha\cos\beta x \sin(y - y_0) = 0, \tag{A.1}$$

$$\sin\beta x \cos(y - y_0) = 0. \tag{A.2}$$

We define Y as the set of points (x,y) where U attains its global minimum $U_{\min}$. We also define the sets

$$V_\pm = \{y\colon\ y \pm \alpha\sin(y - y_0) = 0,\ \pm\cos(y - y_0) > 0\},$$

$$W_+ = \{(0,y)\colon\ y \in V_+\}, \qquad W_- = \left\{\left(\frac{\pi}{\beta}, y\right)\colon\ y \in V_-\right\}$$

and set $y_* = \min_{y\in V_+\cup V_-}|y|$.

Lemma 1. *We have*

$$Y = \{(0,y)\colon\ |y| = y_*,\ y \in V_+\} \cup \left\{\left(\frac{\pi}{\beta}, y\right)\colon\ |y| = y_*,\ y \in V_-\right\}.$$

Proof. We seek the global minimum among the critical points. It follows from (27) that $\sin x = 0$ (because $U \ge 0$ if $\cos(y - y_0) = 0$). It is obvious from (26) that all critical points such that $U < 0$ belong to $W_+ \cup W_-$. Further,

$$U(x,y) = \frac{y^2}{2} - \sqrt{\alpha^2 - y^2} \quad \forall\,(x,y) \in W_+ \cup W_-.$$

Hence, the closer y is to zero, the less U is. ■

Lemma 2. *There exists at most one $y \in V_+$ such that $|y| = y_*$. The same holds for V_-.*

Proof. We suppose the contrary, i.e., $\pm y_* \in V_+$. We then have

$$\pm y_* + \alpha\sin(\pm y_* - y_0) = 0, \qquad \cos(\pm y_* - y_0) > 0,$$

or summing the equalities, we obtain

$$\sin(y_* - y_0) - \sin(y_* + y_0) = -2\sin y_0 \cos y_* = 0.$$

Hence, either $y_0 = 0$ (then, obviously, $y_* = 0$) or $y_* = \pi/2 + \pi n$. In the latter case, we obtain simultaneously $\sin y_0 > 0$ and $\sin y_0 < 0$, which is a contradiction. ■

Lemma 3. *We have $V_- \cap V_+ = \varnothing$.*

Proof. Otherwise, $\cos(y_* - y_0)$ is simultaneously negative and positive. ■

It follows from the proved lemmas that Y contains either one or two elements. In the latter case, we have only one remaining possibility: $Y = \{(0, \pm y_*), (0, \mp y_*)\}$. Then

$$\pm y_* \pm \alpha \sin(\pm y_* - y_0) = 0, \qquad \pm \cos(\pm y_* - y_0) > 0,$$

or $\sin y_* \cos y_0 = 0$, whence $\cos y_0 = 0$. Indeed, $y_* = \pi n$ is impossible because $\cos(\pi n - y_0) = \cos(-\pi n - y_0)$. Hence, $y_0 = \pi/2$.

Proposition 1 is proved.

Appendix B: Proposition 3: The idea of the proof

1. The assertion in point 1 is obvious because $v(x)$ is also an even function.
2. The assertion in point 2 follows from the representation

$$\zeta^m(x) = \frac{1}{2\pi} \int_0^1 \Theta^m(x, q) e^{iqx}\, dq,$$

where $\Theta^m(x, q) = \Phi^m(x, q)e^{-iqx}$ is 2π-periodic in x. Using integration by parts, we can now see that $\zeta^m(x) = O(1/x^\infty)$.

3. To prove the assertion in point 3, we substitute expansion (20) and the energy expansion

$$E_m(q) = \sum_{l \in \mathbb{Z}} \varepsilon_l^m e^{2\pi i l q}$$

in the Schrödinger equation and obtain the relations

$$\widehat{H} c_k(x) = \sum_{l+s=k} \varepsilon_l^m c_s. \tag{A.3}$$

But because the band widths are exponentially small, all ε_l for $l \neq 0$ are also exponentially small. Therefore, we can write the approximation

$$\widehat{H} c_k(x) \approx \varepsilon_0^m c_k$$

with an exponentially small error, and c_k are hence quasimodes of $\widehat{H}$.

Appendix C: Proposition 4: The idea of the proof

To calculate asymptotic approximation for the band widths, we need a good approximation for the Wannier function ζ_0^m only on the segment $-\pi \le x \le \pi$. We multiply ζ_0^m by a smooth cutoff function χ_0 with the support $[-2\delta - \pi, \pi + 2\delta]$ and equal to 1 for $-\delta - \pi \le x \le \pi + \delta$ (the obtained function is again denoted by ζ_0^m). This operation does not change the leading term of the asymptotic approximation. Hence, expansion (21) admits the approximation

$$\Phi^m(x, q) = \zeta_0^m(x) + \zeta_0^m(x - 2\pi)e^{2\pi i q} + \zeta_0^m(x + 2\pi)e^{-2\pi i q} \tag{A.4}$$

for $x \in [-\pi, \pi]$.

To simplify the notation in what follows, we write $\Phi(q)$, ζ_0, and $E(q)$ instead of $\Phi^m(x, q)$, ζ_0^m and $E_m(q)$. Using the Herring approach, we integrate the identity

$$-\frac{h^2}{2}(\Phi(0)\Delta\Phi(q) - \Phi(q)\Delta\Phi(0)) = (E(q) - E(0))\Phi(q)\Phi(0)$$

in the limits $-\pi \le x \le \pi$ and then by the Green formula obtain

$$E(q) - E(0) = -\frac{h^2(\Phi(0)\Phi(q)' - \Phi(q)\Phi(0)')|_{-\pi}^{\pi}}{2\int_{-\pi}^{\pi} \Phi(0)\Phi(q)\,dx}. \tag{A.5}$$

Because $\Phi(q)$ are localized near $x = 0$, the denominator is obviously close to unity. We define

$$\zeta_+ = \zeta_0^m(\pi), \qquad \zeta_- = \zeta_0^m(-\pi), \qquad \zeta_+' = (\zeta_0^m)'(\pi), \qquad \zeta_-' = (\zeta_0^m)'(-\pi).$$

Substituting (29) in (30), we obtain

$$\begin{aligned} E(q) - E(0) \sim\ & -\frac{h^2}{2}[(\zeta_+ + \zeta_-)(\zeta_+' + \zeta_-' e^{2\pi i q}) - (\zeta_+ + \zeta_- e^{2\pi i q})(\zeta_+' + \zeta_-') + \\ & + (\zeta_- + \zeta_+)(\zeta_-' + \zeta_+' e^{-2\pi i q}) + (\zeta_- + \zeta_+ e^{-2\pi i q})(\zeta_-' + \zeta_+')]. \end{aligned} \tag{A.6}$$

Clearly, $\zeta_+ = \zeta_-$ and $\zeta_+' = -\zeta_-'$, and we obtain the required relation (22).

Appendix D: One-dimensional case without the symmetry $x \to -x$

We apply Theorem 6 to operator (5) on the circle $x \pmod{4\pi}$. The eigenvalues of P are then $E_0(0)$ and $E_0(1/2)$, and because of the symmetry $x \to x + 2\pi$, we have

$$E_0(0) = \mathcal{E} + w_{1\,2} + O\left(-\frac{2\sigma}{h}\right), \qquad E_0\left(\frac{1}{2}\right) = \mathcal{E} - w_{1\,2} + O\left(-\frac{2\sigma}{h}\right)$$

(because the periodic and antiperiodic eigenfunctions correspond to the eigenvectors of P respectively close to $(1,1)$ and $(1,-1)$).

The problem thus reduces to finding an asymptotic approximation for $w = w_{1\,2}$:

$$w = \frac{h^2}{2}(\psi_1\psi_2' - \psi_2\psi_1')|_a^b, \quad -2\pi < b < 0 < a < 2\pi. \tag{A.7}$$

We can obtain it by substituting the WKB approximation for ψ_j in (32). Namely, for $j = 1, 2$, we take $\phi_j(x) = h^{-1/4}A_j(x)e^{-S_j(x)/h}$, where $S_j(x) = d(z_j, x)$ and A_j is found from the transport equation

$$\frac{dA_j}{dx} + \frac{A_j S''}{2} = \frac{\omega}{2}A_j. \tag{A.8}$$

We define $\widetilde{w}_{a,b} = (h^2/2)(\phi_1\phi_2' - \phi_2\phi_1')|_{a,b}$ and calculate $\widetilde{w} = \widetilde{w}_b$. We assume that $x = x_0(t)$ is the instanton parameterized as

$$x_0 \to 0, \quad t \to -\infty, \qquad x_0(t) \to 2\pi, \quad t \to +\infty, \qquad x_0(0) = b.$$

Then

$$|\widetilde{w}| = h^{1/2}A_1(x_0(0))A_2(x_0(0))|\dot{x}_0(0)|e^{-\sigma_0/h}(1 + o(1)), \quad h \to 0, \tag{A.9}$$

where σ_0 is the Jacobi length of the instanton. We also define $a_j(t) = A_j(x_0(t))$.

Proposition 5. *We have the asymptotic approximation*

$$|\widetilde{w}| = \left(\frac{h\omega\gamma_-\gamma_+}{\pi}\right)^{1/2} e^{-\sigma_0/h}(1 + o(1)), \quad h \to 0,$$

where $\gamma_\pm = \lim_{t\to\pm\infty} |\dot{x}_0(t)|e^{\mp\omega t}$.

Proof. It follows from (33) that

$$a_1(t) = a_1(0)\exp\left[-\frac{1}{2}\int_0^t S''(x_0(\tau))\,d\tau\right]e^{-\omega t/2} = a_1(0)\left|\frac{\dot{x}_0(0)}{\dot{x}_0(t)}\right|^{1/2} e^{-\omega t/2},$$

and from the harmonic oscillator approximation, $\lim_{t\to-\infty} a_1(t) = (\omega/\pi)^{1/4}$, whence we obtain

$$a_1(0) = \left(\frac{\omega}{\pi\dot{x}_0^2}\right)^{1/4}\sqrt{\gamma_-}.$$

Similar calculations for $a_2(0)$ finish the proof. ■

The next step is to substitute the action $S_{h,0}$ given by (9) in the exponent. It was shown in [11] that

$$\sigma_0 = S_{h,0} + \frac{h}{2} + h\log 2 + \frac{h\omega(T_h^- + T_h^+)}{2} + o(h),$$

where $T_h^\pm > 0$ is the time of movement along the instanton $x_0(t)$ from the point $x_\pm(h,0)$ to b (see (9)).

Therefore,

$$|\widetilde{w}| = \frac{1}{2}\left(\frac{h\omega\gamma_-\gamma_+}{\pi e}\right)^{1/2} e^{\omega(T_h^- + T_h^+)/2} e^{-S_{h,0}/h}(1 + o(1)).$$

Further,

$$\gamma_\pm = \lim_{\varepsilon\to 0} e^{\omega T^\pm(\varepsilon)}|\dot{x}_0(T^\pm(\varepsilon))| = \lim_{\varepsilon\to 0} e^{\omega T^\pm(\varepsilon)}\sqrt{2\varepsilon},$$

where $T^\pm(\varepsilon) = T^\pm_{2\varepsilon/\omega}$. Hence,

$$e^{\omega T_h^\pm} = \frac{\gamma_\pm}{\sqrt{\omega h}}(1 + o(1)),$$

and finally

$$|\widetilde{w}_b| = \frac{\omega h}{2\sqrt{\pi e}} e^{-S_{h,0}/h}(1 + o(1)).$$

A similar formula holds for $\widetilde{w}_a$, and

$$\widetilde{w}_b - \widetilde{w}_a = b_0\frac{\omega h}{\pi} e^{-S_{h,0}/h}(1 + o(1)), \tag{A.10}$$

where b_0 is given by (17).

To prove that the right-hand side of (35) gives a correct asymptotic approximation for w, we note that

$$\psi_j(x) = \phi(x) + O(h^{3/4}e^{-S_j(x)/h}), \qquad \psi_j'(x) = \phi'(x) + O(h^{-1/4}e^{-S_j(x)/h})$$

uniformly in x (see [3]). Hence, asymptotic approximation (34) also holds for ψ_1 and ψ_2. Theorem 1 is thus proved for $m = 0$ and $q = 1/2$.

Appendix E: Proofs of Theorems 4 and 5

We first study eigenfunctions periodic and antiperiodic in x. The potential U on the cylinder $Z_{(2)}$ has four wells denoted by

$$z_1 = (0, y_*), \qquad z_2 = (\pi, -y_*), \qquad z_3 = (2\pi, y_*), \qquad z_4 = (3\pi, -y_*).$$

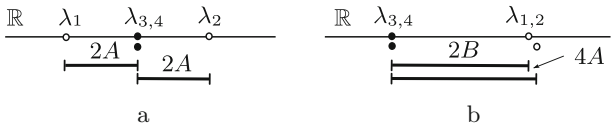


Fig. 10. Spectral bands in Case 2: the white and black dots are the respective periodic and antiperiodic states. The bands (a) have the widths $2A$ and are adjacent if $d_{\text{het}} < d_{\text{hom}}$ and (b) overlap and have the widths $2B$ if $d_{\text{hom}} < d_{\text{het}}$.

We set $A = w_{1\,2}$ and $B = w_{1\,3}$. The leading term of the matrix P is then equal to

$$W = \begin{pmatrix} \mathcal{E} & A & B & A \\ A & \mathcal{E} & A & B \\ B & A & \mathcal{E} & A \\ A & B & A & \mathcal{E} \end{pmatrix}, \tag{A.11}$$

and the eigenvalues and eigenvectors are hence

$$\begin{aligned} &\lambda_1 = \mathcal{E} - B + 2A, \qquad && v_1 = (1,1,1,1), \\ &\lambda_2 = \mathcal{E} - B - 2A, \qquad && v_2 = (1,-1,1,-1), \\ &\lambda_{3,4} = \mathcal{E} + B, \qquad && v_3, v_4 \in \operatorname{Span}((1,0,-1,0),(0,1,0,-1)). \end{aligned} \tag{A.12}$$

We prove that the eigenvalues of P corresponding to $\lambda_{3,4}$ are exactly degenerate. We introduce a symmetry operator $G_1\psi(x,y) = \psi(x+\pi,-y)$. Obviously, $\widehat{H}$ commutes with G_1, and $G_1^4 = \mathrm{Id}$. As before, we decompose the four-dimensional space $\mathcal{V}$ into a direct sum of $\widehat{H}$-invariant subspaces $\mathcal{V}^{(j)}$, $j = 0,1,2$. They are two one-dimensional spaces $\mathcal{V}^{(0)}$ and $\mathcal{V}^{(1)}$ associated with λ_1 and λ_2, and also two-dimensional $\mathcal{V}^{(2)}$ associated with $\lambda_{3,4}$. The spaces $\mathcal{V}^{(j)}$ are also G_1-invariant.

Therefore, from (37) and Remark 12, we easily find that $\mathcal{V}^{(j)}$, $j = 0,1$, are generated by $\psi_{1,2}$ such that $G_1\psi_1 = \psi_1$ and $G_1\psi_2 = -\psi_2$. Both functions are Bloch functions with the quasimomentum $q = 0$.

Because the subspace in $\mathcal{V}$ generated by Bloch functions with $q = 0$ is two-dimensional, the eigenvalues of $G_1|_{\mathcal{V}^{(2)}}$ are $\pm i$. Hence, $\mathcal{V}^{(2)}$ corresponds to a multiplicity-two eigenvalue (the quasimomentum is $q = 1/2$).

Case $d_{\text{het}} < d_{\text{hom}}$. We take $\sigma = d_{\text{het}}/2$. Then $B = 0$, and from Remark 12, we can see that the highest and lowest eigenstates $\lambda_{1,2}$ are associated with $q = 0$, and a double eigenvalue $\lambda_{3,4}$ in the middle is associated with $q = 1/2$ (see Fig. 10a). The differences $|\lambda_{1,2} - \lambda_{3,4}|$ are equal to $2A \sim e^{-d_{\text{het}}/h}$ and are reducible to the same integral as in Theorem 3. Therefore, A admits the asymptotic approximation from the right-hand side of (16).

In a more general formulation, we seek Bloch eigenfunctions with rational quasimomenta $q = k/2n$, where $k = 0,\dots,2n-1$. In other words, we study $4n$ eigenfunctions of $\widehat{H}$ on the cylinder $Z_{(2n)}$. In Theorem 6, we can then take $W = A\Omega_{4n}$ (see (24)). Its eigenvectors and eigenvalues,

$$v_k = (1, e^{\pi i k/2n}, e^{2\pi i k/2n}, \dots, e^{\pi i k(4n-1)/2n}), \qquad \lambda_k = 2A\cos\frac{\pi k}{2n},$$

imply dispersion relation (18).

Theorem 4 is thus proved.

Case $d_{\text{hom}} < d_{\text{het}}$. We take $\sigma = d_{\text{hom}}/2$ and again start with $Z_{(2)}$. In (36), we then have $A = 0$, and from (37) according to Remark 12, we have a pair of periodic states $\lambda_{1,2}$ and a double antiperiodic state

$\lambda_{3,4}$. The difference $|\lambda_{1,2} - \lambda_{3,4}| \sim 2B$. Also, taking $\sigma = d_{\text{hom}}/2\text{m}$ we can easily calculate $|\lambda_1 - \lambda_2| \sim 4A$ (see Fig. 10b).

Again, we seek Bloch functions with rational quasimomenta: $q = k/2n$, where $k = 0, \ldots, 2n-1$. The operator W in Theorem 6 now has two $2n$-dimensional invariant subspaces (associated with odd and even elements). On each space, W is determined by the matrix $B\Omega_{2n}$, which was studied previously.

Dispersion relation (19) hence easily follows. Theorem 5 is proved.

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