Semiclassical Limits of the Spectrum of Harper's Equation

Michael Wilkinson and Ritchie J. Kay
Department of Physics and Applied Physics, John Anderson Building, University of Strathclyde, Glasgow G4 0NG, United Kingdom
(Received 18 August 1995)

Harper's equation, a model for magnetic field effects in lattices, can be analyzed using semiclassical methods when the commensurability parameter β is small. We discuss an effective Hamiltonian $\hat{H}_{\rm eff}$ describing a subset of the spectrum, for which the rational limit $\beta \longrightarrow p/q$ is also a semiclassical limit; we give the first two terms of the expansion of $\hat{H}_{\rm eff}$ in powers of $\beta - p/q$. We derive a Bohr-Sommerfeld quantization condition, involving a Berry phase correction, and an equation for the bandwidth when $\beta = p_1/q_1$ with q_1 large. We also discuss the dynamics of $\hat{H}_{\rm eff}$ under infinitesimal gauge transformations of the rational Bloch states.

PACS numbers: 71.10.Fd, 03.65.Sq

Harper's equation

$$\psi_{n+1} + \psi_{n-1} + 2\cos(2\pi\beta n + \delta)\psi_n = E\psi_n \tag{1}$$

is a discrete Schrödinger equation which is widely used as a model for electrons in two-dimensional lattice structures penetrated by a magnetic field, or for electrons in incommensurate potentials. The parameter β is the ratio of the area of a flux quantum to that of the unit cell, or the commensurability of the superposed potentials: Derivations of the Harper equation in the context of Bloch electrons in a magnetic field are given in [1,2]. The solution of (1) for the energy levels E and eigenstates $\{\psi_n\}$ is a difficult problem for which semiclassical methods have been very useful [3,4]; the semiclassical limit is $\beta \longrightarrow 0$, and we define a dimensionless effective Planck constant $\hbar = 2\pi\beta$. For many purposes this limit is sufficient for physical applications; for example, in ordinary solids the number of flux quanta per unit cell is always small. Experiments on artificial lattices make values of β of order unity achievable, and distinctive features of the spectrum of Harper's equation may soon be detectable in semiconductor superlattices [5], and in superconducting grids [6]. In this Letter we discuss an effective Hamiltonian method for which the semiclassical limit is $\beta \longrightarrow p/q$ (p and q are coprime integers): Because the rationals are a dense set, this provides a far-reaching extension of the semiclassical approach. The idea that $\beta \longrightarrow p/q$ can be a semiclassical limit was originally proposed by Sokoloff [7], and later developed by others [8–10]; we will give simple derivations of results which cannot be obtained using these earlier approaches.

When $\beta = p/q$, the eigenstates of (1) are Bloch waves, and the spectrum consists of q bands. We will describe an effective Hamiltonian for a subset of the spectrum which collapses onto a Bloch band as $\beta \longrightarrow p/q$; because the effective Hamiltonian is similar in form to the original one, this is a renormalization group (RG) transformation. The results are obtained from an algorithm for constructing an exact effective Hamiltonian derived in [11], following an approach introduced in [12]. This Letter gives explicit expressions for the first two terms of a series expansion in $\Delta\beta = \beta - p/q$. The zeroth order term was deduced in the earlier papers, but this is not sufficient to determine the spectrum in the limit $\beta \longrightarrow p/q$, because the first order correction is required for the Bohr-Sommerfeld quantization condition. With the addition of the first order correction, the RG method gives a satisfying understanding of the spectrum of Harper's equation.

Our expression for the first order term is written in terms of the rational Bloch eigenstates: It consists of two components, one of which is not invariant under "gauge transformations" which alter the relative phases of the Bloch states at different points in the Brillouin zone. We write the Bohr-Sommerfeld quantization condition in gauge invariant form by incorporating the contribution from the gauge dependent term as a Berry phase correction; a related expression was obtained by Chang and Niu [13], but their calculation misses the gauge independent first order contribution. We also apply the first order correction to a calculation of the total width of the spectrum of the band when $\beta = p_1/q_1$, which is a high order rational approximant of p/q. We will derive a formula recently proposed by Tan [14] on the basis of numerical experiments; efforts to derive this result using the methods of [8–10] were not successful. We anticipate that our results will find other applications, for example, in problems involving the total energy of the Harper spectrum [15].

The Hamiltonian of Harper's equation is a special case of

$$\begin{aligned} \hat{H} &= \sum_{nm} H_{nm}\hat{T}(n\hbar, m\hbar), \\ \hat{T}(X,P) &= \exp[i(P\hat{x} - X\hat{p})/\hbar], \end{aligned} \tag{2}$$

where $H_{-n,-m} = H^*_{nm}$, and the operator $\hat{T}(X,P)$ is a phase-space translation operator. In Harper's equation the only nonzero coefficients of (2) are $H_{10} = H_{01} = 1$ (and their symmetry related images). Our results will apply to the more general Hamiltonian (2), unless otherwise stated. The translation operators $\hat{T}(X,P)$ have a noncommutative algebra which is isomorphic to that of the "magnetic translation group" describing an electron moving in a plane with a perpendicular magnetic field [16].

When β is rational, the solution of the Schrödinger equation corresponding to (2) is a Bloch wave, which we will denote by $|B_\nu(k,\delta)\rangle$, and which we can write in the form

$$\langle x|B_\nu(k,\delta)\rangle = \sum_n \exp(ikx/\hbar)\, u_n(k,\delta)\, \delta(x - n\hbar - \delta)\,, \tag{3}$$

where the vector $\{u_n\}$ is periodic: $u_n = u_{n+q}$. The q distinct elements of the periodic vector $\{u_n\}$ can be obtained as an eigenvector of a $q \times q$ matrix $\tilde{H}(k,\delta)$ with elements

$$[\tilde{H}(k,\delta)]_{nm} = \sum_M H_{n-m,M} \exp[-ik(n-m)] \times \exp\Big[iM\Big(\delta + \tfrac{1}{2}(n+m)\hbar\Big)\Big] \tag{4}$$

and the eigenvalues $\mathcal{E}_\nu(k,\delta)$, $\nu = 1,\ldots,q$, are the dispersion relations of the Bloch bands. We will use the notation $|u_\nu(k,\delta))$ for the q-dimensional eigenvectors of this matrix, and we denote Dirac brackets in the Hilbert space of q-dimensional vectors by $(a|b)$. The phases of the Bloch states can be chosen so that

$$|B_\nu(k,\delta + 2\pi p/q)\rangle = |B_\nu(k,\delta)\rangle,$$
$$|B_\nu(k + 2\pi/q,\delta)\rangle = \exp[iqM_\nu\delta/p]\,|B_\nu(k,\delta)\rangle, \tag{5}$$

where M_ν is an integer called the Chern number; Thouless *et al.* [16] showed that M_ν is the quantized Hall conductance integer of the band. A conjugate integer N_ν, given by $pN_\nu + qM_\nu = 1$, will also play an important role in the theory.

The effective Hamiltonian $\hat{H}^{(\nu)}_{\rm eff}$, describing the subset of the spectrum which collapses onto the νth Bloch band in the rational limit, is expanded as a power series in $\Delta\hbar = 2\pi(\beta - p/q)$:

$$\hat{H}^{(\nu)}_{\rm eff} = \hat{H}^{(\nu)}_0 + \Delta\hbar \hat{H}^{(\nu)}_1 + O(\Delta\hbar^2)\,. \tag{6}$$

The contributions $\hat{H}^{(\nu)}_i$ are periodic functions of operators $\hat{x}'$ and $\hat{p}'$ which have a renormalized commutator: $[\hat{x}',\hat{p}'] = i\hbar'_\nu$. In [11] and [12], it was shown that the zeroth order term is obtained by quantizing the dispersion relation $\mathcal{E}_\nu(k,\delta)$: $\hat{H}^{(\nu)}_0 = \mathcal{E}_\nu(\hat{x}'/q,\hat{p}'/q)$, where periodic functions are understood to be quantized by evaluating their Fourier coefficients and associating them with an operator using an expansion of the form (2). The formula for the renormalization of $\hbar$ depends on the Chern integer M_ν of the band:

$$\hbar'_\nu = 2\pi\beta'_\nu, \quad \beta'_\nu = \frac{q\beta - p}{\beta N_\nu + M_\nu}\,. \tag{7}$$

We find that $\hat{H}^{(\nu)}_1$ is obtained by quantizing a function $H^{(\nu)}_1(k,\delta)$ by the substitutions $k \to \hat{x}'/q$, $\delta \longrightarrow \hat{p}'/q$: We write $H^{(\nu)}_1(k,\delta) = H^{(\nu)}_{1a}(k,\delta) + H^{(\nu)}_{1b}(k,\delta)$, where

$$H^{(\nu)}_{1a}(k,\delta) = \frac{i}{2}\left[\left(\frac{\partial u_\nu}{\partial\delta}\,\middle|\,\mathcal{E}_\nu(k,\delta) - \tilde{H}(k,\delta)\,\middle|\,\frac{\partial u_\nu}{\partial k}\right) - \left(\frac{\partial u_\nu}{\partial k}\,\middle|\,\mathcal{E}_\nu(k,\delta) - \tilde{H}(k,\delta)\,\middle|\,\frac{\partial u_\nu}{\partial\delta}\right)\right],$$
$$H^{(\nu)}_{1b}(k,\delta) = i\left(u_\nu\,\middle|\,\frac{\partial u_\nu}{\partial k}\right)\frac{\partial\mathcal{E}_\nu}{\partial\delta} - i\left(u_\nu\,\middle|\,\frac{\partial u_\nu}{\partial\delta}\right)\frac{\partial\mathcal{E}_\nu}{\partial k} + \frac{kqN_\nu}{2\pi}\frac{\partial\mathcal{E}_\nu}{\partial k}\,. \tag{8}$$

The expression $H^{(\nu)}_{1a}$ in (8) was previously discovered by Rammal and Bellissard [9] as the first order correction to the effective Hamiltonian at the extremum of a band; their approach only assigns a meaning to $H^{(\nu)}_{1a}$ at the extrema. The term $H^{(\nu)}_{1b}$ vanishes at the stationary points of the dispersion relation, and does not therefore invalidate the result of [9].

The vector $|u_\nu(k,\delta))$ is assumed to be an analytic function of k and δ. It can be subjected to a gauge transformation by multiplying by a factor $\exp[i\theta(k,\delta)]$. The expression $H^{(\nu)}_{1a}$ is gauge invariant, whereas $H^{(\nu)}_{1b}$ is not. The effect of an infinitesimal gauge transformation with phase $\theta(k,\delta)d\tau$, periodic on the Brillouin zone, is to transform the Hamiltonian from H to H':

$$H' = H + \hbar'_\nu\{H,\theta\}d\tau + O(d\tau^2) + O(\Delta\hbar^2)\,, \tag{9}$$

where we use $p' = qk$, $x' = q\delta$, and $\{A,B\}$ is the Poisson bracket $\partial_{x'}A\partial_{p'}B - \partial_{x'}B\partial_{p'}A$. This is the equation for an infinitesimal canonical transformation generated by the Hamiltonian $\hbar'_\nu\theta(k,\delta) + O(\hbar'_\nu)$ acting for a time $d\tau$. To leading order in $\hbar'$, the Poisson bracket in (9) can be replaced by a commutator; (9) therefore also corresponds to an infinitesimal unitary transformation, generated by a "gauge Hamiltonian" $\hat{G} = \hbar'_\nu\theta(\hat{x}'/q,\hat{p}'/q)$, acting for time $d\tau$. Because unitary evolution of an observable leaves its eigenvalues unchanged, the gauge transformation does not alter the spectrum of the effective Hamiltonian.

The form of $H^{(\nu)}_{1b}$ given in (8) is not precisely symmetric between k and δ; this is a consequence of constraints on the gauge of the Bloch waves which are implied by (5). Allowing for a more general gauge transformation of the vectors $|u_\nu(k,\delta))$, we can write this term in a symmetric form

$$H_{1b}^{(\nu)}(k,\delta) = \mathbf{A} \wedge \nabla \mathcal{E}_\nu(k,\delta)\,, \tag{10}$$

where $\mathbf{A} = i(u_\nu|\nabla u_\nu) + \mathbf{A}'$, ∇ represents a vector operator $(\frac{\partial}{\partial k}, \frac{\partial}{\partial \delta})$, and $\mathbf{A}'$ is chosen such that $\mathbf{A}$ is periodic, and the integral of $\nabla \wedge \mathbf{A}$ over the Brillouin zone vanishes.

Before discussing the applications of these results, we give a brief sketch of the method by which they are obtained; a detailed derivation will be published separately [18]. We calculate the effective Hamiltonian and normalization operators, which have the same matrix elements as (2) when expressed in a suitable basis [12]. The Hamiltonian operator, $\hat{H}'_\nu$, is of the same form as (2) with Fourier coefficients $H_{nm}^{(\nu)}$ and commutator $[\hat{x}', \hat{p}'] = i\hbar'_\nu$, and the normalization operator is similar, with coefficients $N_{nm}^{(\nu)}$. In terms of these operators, the Schrödinger equation takes the form $(\hat{H}'_\nu - E\hat{N}'_\nu)|\psi\rangle = 0$. It is possible to transform $\hat{H}'_\nu$ to an orthonormal basis by multiplying from the left by $(\hat{N}'_\nu)^{-1}$, to produce an effective Hamiltonian $\hat{H}_{\text{eff}}^{(\nu)} = (\hat{N}'_\nu)^{-1}\hat{H}'_\nu$. The formula for the Fourier coefficients $H_{nm}^{(\nu)}$ of the effective Hamiltonian (6) was obtained in [11]; they are given by a linear transformation of the Fourier coefficients of the original Hamiltonian

$$H_{nm}^{(\nu)} = \sum_N \sum_M H_{NM} \tau_{nm}^{NM} \tag{11}$$

and the $N_{nm}^{(\nu)}$ are obtained by replacing H_{nm} by $\delta_{n0}\delta_{m0}$. The coefficients τ_{nm}^{NM} are obtained from a set of N_ν generalized Wannier functions: Although $|B_\nu(k,\delta)\rangle$ cannot be made periodic in k and δ (except when $M_\nu = 0$), a gauge can be chosen such that the vector $|C_\nu(k,\delta)\rangle = \hat{T}(0, -qM_\nu k)\,|B_\nu(k,\delta)\rangle$ is periodic. The generalized Wannier functions $|\phi_\mu^{(\nu)}\rangle$, $\mu = 1,\ldots,N_\nu$, are then obtained by integrating over the Bloch wave vectors as follows:

$$|\phi_\mu^{(\nu)}\rangle = \frac{1}{N_\nu} \sum_{\lambda=1}^{N_\nu} \exp[2\pi i\mu\lambda/N_\nu]\hat{T}_0(2\pi\lambda/N_\nu, 0) \times \int_0^{2\pi/q} dk \int_0^{2\pi p/q} d\delta\, \exp[iqk\lambda]\,|C_\nu(k,\delta)\rangle \tag{12}$$

(the subscript 0 on the $\hat{T}$ operator implies that it is evaluated setting $\hbar = \hbar_0 \equiv 2\pi p/q$). The coefficients τ_{nm}^{NM} are given in [11]:

$$\tau_{nm}^{NM} = (-1)^{(nN+mM-nmq)p} \sum_{\mu=1}^{N_\nu} \langle \phi_\mu^{(\nu)}|\hat{P}\hat{\tau}_{nm}^{NM}\hat{P}|\phi_\mu^{(\nu)}\rangle,$$
$$\hat{\tau}_{nm}^{NM} = \hat{t}(M - nq, N - mq) \times \hat{T}\big((-2\pi m + N\kappa_\nu)/N_\nu, (-2\pi n + M\kappa_\nu)\hbar/\kappa_\nu\big)\,. \tag{13}$$

In this expression $\kappa_\nu = 2\pi M_\nu + N_\nu \hbar$, $\hat{P}$ is a projection operator for the νth band of the Hamiltonian, and the operator $\hat{t}(\lambda_1, \lambda_2)$ is defined by the relation

$$\hat{t}(\lambda_1,\lambda_2)\,|\phi_\mu^{(\nu)}\rangle = \exp\Big[2\pi i M_\nu\Big(\mu - \tfrac{1}{2}\lambda_1\Big)\lambda_2/N_\nu\Big] \times |\phi_{\mu-\lambda_1}^{(\nu)}\rangle\,. \tag{14}$$

We wish to expand the Fourier coefficients (11) to first order in $\Delta\hbar$ around the rational value $\hbar_0 = 2\pi p/q$. Because the derivative with respect to $\hbar$ of the translation operator $\hat{T}(X,P)$ in (13) contains factors proportional to $\hat{x}$ and $\hat{p}$, we require matrix elements of the form $\langle \phi_\mu^{(\nu)}|\hat{p}\hat{T}(X,P)|\phi_{\mu'}^{(\nu)}\rangle$ (and similarly for $\hat{x}$): They can be obtained from the matrix elements $\langle B_\nu(k',\delta')|\hat{p}|B_\nu(k,\delta)\rangle = p(k,k',\delta,\delta')$ by integration over k, δ, k', and δ' using (12). These matrix elements can be calculated in terms of the vectors $|u_\nu(k,\delta)\rangle$: We find for the matrix elements of $\hat{p}$

$$p(k,k',\delta,\delta') = i\hbar\frac{\partial}{\partial\delta}\{\delta(\delta-\delta')\delta(k-k')\exp[i(k\delta - k'\delta')/\hbar]\} + \delta(\delta-\delta')\delta(k-k')\Big[k - i\hbar\Big(u_\nu(k,\delta)\,\Big|\,\frac{\partial u_\nu}{\partial\delta}(k,\delta)\Big)\Big]. \tag{15}$$

The matrix elements of $\hat{x}$ are obtained by deleting the term proportional to k, then replacing $p \leftrightarrow x$, $k \leftrightarrow -\delta$. After a lengthy calculation, we determine the first order correction in the form (8).

We will now describe two results which use (8) in a semiclassical context. First we consider the Bohr-Sommerfeld quantization rule, which describes the spectrum in the semiclassical limit $\beta \to p/q$. The Bohr-Sommerfeld condition is an implicit equation for the energy level E_n within the νth band:

$$S(E_n) = \oint_{H_{\text{eff}}^{(\nu)}=E_n} p'\,dx' = 2\pi\Big(n + \tfrac{1}{2}\Big)\hbar'_\nu + O(\hbar'^2_\nu)\,. \tag{16}$$

This equation can be written in gauge invariant form by incorporating the gauge dependent term as a phase correction γ:

$$S_{\text{inv}}(E_n) = \oint_{H_{\text{inv}}=E_n} p'\,dx' = 2\pi\Big(n + \tfrac{1}{2} + \gamma\Big)\hbar'_\nu + O(\hbar'^2_\nu)\,, \tag{17}$$

where S_{inv} and $H_{\text{inv}} = H_0^{(\nu)} + \Delta\hbar H_{1a}^{(\nu)}$ are the gauge invariant parts of the action and Hamiltonian, and (in the case where the contour encloses a minimum of $H_{\rm eff}^{(\nu)}$)

$$\gamma = -\frac{1}{2\pi}\frac{\partial(S - S')}{\partial\hbar'_\nu}\bigg|_{E_n} = \frac{1}{q^2}\oint_{H_0^{(\nu)}=E_n} ds\frac{H_{1b}^{(\nu)}}{|\nabla' H_0^{(\nu)}|}\,. \tag{18}$$

Here ds is a Euclidean distance element of a contour around the path $H_{\rm inv}(x', p') = E_n$ in phase space, and $\nabla' = (\partial/\partial x', \partial/\partial p')$. We obtain γ in gauge invariant form by converting it to an area integral using (10):

$$\gamma = \frac{1}{q^2}\oint_{H_0^{(\nu)}=E_n} ds\frac{\mathbf{A}\wedge\nabla H_0^{(\nu)}}{|\nabla' H_0^{(\nu)}|} = \frac{1}{q}\oint_{H_0^{(\nu)}=E_n} d\mathbf{l}\cdot\mathbf{A} = \int dk\int d\delta\,\Theta\big(E_n - \mathcal{E}_\nu(k,\delta)\big)\left(V_\nu - \frac{qN_\nu}{2\pi}\right), \tag{19}$$

where $d\mathbf{l}$ is a line element of the clockwise contour $H_0^{(\nu)}(x', p') = E_n$, $\Theta(x)$ is the unit increasing step function, and V_ν is the Berry phase two-form,

$$V_\nu(k,\delta) = i\left[\left(\frac{\partial u_\nu}{\partial k}\,\bigg|\,\frac{\partial u_\nu}{\partial\delta}\right) - \left(\frac{\partial u_\nu}{\partial\delta}\,\bigg|\,\frac{\partial u_\nu}{\partial k}\right)\right]. \tag{20}$$

In gauge invariant form, the phase correction γ is an area integral, which measures the Berry phase accumulated by the vector $|u_\nu(k,\delta))$ as it is cycled around the phase trajectory, minus a counter term $N_\nu S_{\rm inv}(E_n)/2\pi q = N_\nu(n + \frac{1}{2})\hbar'_\nu/q$. If the contour encloses a maximum of $H_{\rm eff}^{(\nu)}$, the sign of γ is reversed. Our expressions for the Bohr-Sommerfeld quantization are, surprisingly, closely related to results obtained in [10] using a different effective Hamiltonian and a different expression for $\hbar'$.

Finally, we describe another application of our results. If β is a rational number p_1/q_1, then $\beta'_\nu = p'/q'$ is also a rational, and the spectrum of the effective Hamiltonian consists of q' bands. Semiclassical arguments indicate that, if the open contour of the effective Hamiltonian forms a simple lattice, the total width of these bands when q' is large depends upon the curvature C_ν of the effective Hamiltonian at its saddle points [4,19]. The total width W_ν of the νth band satisfies

$$\lim_{q'\to\infty} q' W_\nu = \frac{32C}{\pi}C_\nu\,, \tag{21}$$

where C is Catalan's constant. The canonically invariant expression for the curvature is $C_\nu = \frac{1}{2}\sqrt{-\det(\partial_{ij}^2 H_{\rm eff}^{(\nu)})}$ where $\partial_{ij}^2 H_{\rm eff}^{(\nu)}$ is the Hessian matrix of derivatives of the effective Hamiltonian with respect to x' and p', evaluated at its saddle point. We will discuss the evaluation of the first two terms in an expansion of the curvature in powers of $\Delta\hbar$, for the special case of Harper's equation. Because $\partial^2\mathcal{E}/\partial k\partial\delta$ vanishes at the saddle points, we find

$$C_\nu = \frac{1}{2q^2}|\partial_{kk}^2\mathcal{E}_\nu| + \Delta\hbar\frac{1}{4q^2}\,{\rm sgn}(\partial_{kk}^2\mathcal{E}_\nu)\left[\partial_{kk}^2 H_1^{(\nu)} - \partial_{\delta\delta}^2 H_1^{(\nu)}\right] + O(\Delta\hbar^2)$$
$$= \frac{1}{2q^2}|\partial_{kk}^2\mathcal{E}_\nu| + \Delta\hbar\frac{1}{2q^2}\left[{\rm sgn}(\partial_{kk}^2\mathcal{E}_\nu)\partial_{kk}^2 H_{1a}^{(\nu)} - |\partial_{kk}^2\mathcal{E}_\nu|(V_\nu - qN_\nu/2\pi)\right] + O(\Delta\hbar^2)\,, \tag{22}$$

where ∂_x represents differentiation with respect to x, and all derivatives are evaluated at the saddle point of the effective Hamiltonian. Equation (22) is equivalent to a formula proposed by Tan [14]. To obtain this result we used the fact that, for the Harper model, mixed derivatives of $\mathcal{E}_\nu$ and third derivatives vanish at the saddle point; (22) is not always applicable to the general model (2).

The EPSRC provided financial support for R. J. K., and a research grant, No. GR/H94337.

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