

# Slow non-Hermitian cycling: exact solutions and the Stokes phenomenon

M V Berry<sup>1</sup> and R Uzdin<sup>2</sup>

<sup>1</sup> H H Wills Physics Laboratory, Tyndall Avenue, Bristol BS8 1TL, UK

<sup>2</sup> Department of Physics, Technion—Israel Institute of Technology, Haifa 32000, Israel

E-mail: [asymptotico@physics.bristol.ac.uk](mailto:asymptotico@physics.bristol.ac.uk)

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## Abstract

For non-Hermitian Hamiltonians with an isolated degeneracy ('exceptional point'), a model for cycling around loops that enclose or exclude the degeneracy is solved exactly in terms of Bessel functions. Floquet solutions, returning exactly to their initial states (up to a constant) are found, as well as exact expressions for the adiabatic multipliers when the evolving states are represented as a superposition of eigenstates of the instantaneous Hamiltonian. Adiabatically (i.e. for slow cycles), the multipliers of exponentially subdominant eigenstates can vary wildly, unlike those driven by Hermitian operators, which change little. These variations are explained as an example of the Stokes phenomenon of asymptotics. Improved (superadiabatic) approximations tame the variations of the multipliers but do not eliminate them.

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## 1. Introduction

In the quantum mechanics of systems where some freedoms are ignored, or in more general wave phenomena involving absorption or gain, the Hamiltonian operator governing the evolution of states is not Hermitian [1, 2]. Along with the obvious fact that the eigenvalues need not be real (except in special cases such as operators with PT symmetry [2]) has come a growing focus on the deeper phenomena associated with degeneracies. The simplest situation concerns degeneracies of two states. For a Hermitian operator, a degeneracy is a diabolical point [3], at which the two eigenvalues, regarded as functions of parameters on which the Hamiltonian depends, are connected at the intersection point of a surface in the form of a double cone [4], and the two eigenstates are always orthogonal. By contrast, a degeneracy of a non-Hermitian operator, while still typically of codimension 2, is a branch-point (commonly called an exceptional point [5]), around which each eigenstate transforms into the other ('flip' [6]); at the branch-point, the two eigenstates are parallel and each is self-orthogonal

(see chapter 9 of [1]). Reflecting this mathematical distinction, a number of physical phenomena have been identified ([1, 7] and references therein).

Here we will concentrate on the evolution of states driven by a time-dependent non-Hermitian Hamiltonian which is cycled, by forcing it round a loop in the space of its parameters so as to return to its original form. For the Hermitian case there is the adiabatic theorem [8, 9]: if the cycle is slow, evolving states cling to eigenstates of the instantaneous Hamiltonian, so the probability of transitions between eigenstates is small. For non-Hermitian operators, the situation is more subtle. As has recently been pointed out [6], in addition to the eigenstate ‘flip’ associated with the degeneracy if the loop encloses it, it is common for occupation amplitudes to change drastically around the cycle, in way that is different for the two states.

Our aim is to examine the evolution in the context of an exactly solvable model, which illustrates how the drastic occupancy changes are a consequence of the general Stokes phenomenon [10–12] of asymptotics: variation of the multiplier of a function that is exponentially smaller than its companion. The model (section 2) concerns a cycle involving a single isolated degeneracy. Our model operator is non-symmetric, because for symmetric non-Hermitian operators the degeneracies appear in pairs. Pairs of degeneracies are also inevitable for a non-Hermitian operator generated by perturbing a Hermitian one: an isolated diabolical point splits into two branch-points (a familiar phenomenon in crystal optics, for example [13]—and see section 9). Nevertheless, cycling round an isolated degeneracy seems the simplest case and we learn much by studying it in detail, both for its own sake and as a local model when other degeneracies are far away. Mathematically, our study complements the exactly solvable Rabi [14] and Landau-Majorana-Zener [15–17] models for Hermitian operators.

Section 3 contains the exact solution for the Floquet states, that is, the states which return exactly, up to a constant, after the cycle. The solution corresponds to circular parameter-space loops, but these need not be centred on the degeneracy and need not enclose it. In section 4, we consider evolving states that start in each of the two instantaneous eigenstates, and derive an exact formula for the adiabatic multipliers that describe how closely the evolving states cling to the eigenstates during the evolution and especially at the end of the cycle.

Section 5 contains computations for the simplest case, of parameter-space loops with the degeneracy at the centre. The adiabatic multipliers can vary drastically, and this is connected to the Stokes phenomenon. Section 6 shows how the drastic changes get progressively smoothed when the evolving states are represented by successive higher order (‘superadiabatic’) approximations to the evolution [18–20], rather than the instantaneous eigenstates. The change in one of the multipliers can however not be eliminated completely, and for the optimal superadiabatic approximation, whose order is inversely proportional to the slowness, this is described by the universal error function [21, 22] that characterizes asymptotics more generally.

For excentric loops, the asymptotic analysis is more complicated, and depends on whether the loop encloses (section 7) or excludes (section 8) the degeneracy. In the latter case, we concentrate on the limit of small loops.

The brief section 9 shows that the instantaneous eigenstates of our Hamiltonian with an isolated degeneracy are exact evolving states of a slightly modified Hamiltonian—that is, the adiabatic multipliers remain constant. This ‘transitionless driving’ is an application of recent more general ideas [23–26].

The concluding section 10 contains some suggestions for further theoretical study, and a suggestion for an experiment in which these non-Hermitian adiabatic evolutions could appear as physical phenomena. There are three technical appendices.

## 2. Model for non-Hermitian degeneracy

The model is the obviously non-Hermitian Hamiltonian

$$H(\theta) = i \begin{pmatrix} 0 & 1 \\ z(\theta) & 0 \end{pmatrix}, \quad z(\theta) = x(\theta) + iy(\theta), \quad z(\theta + 2\pi) = z(\theta), \quad (2.1)$$

cycled round a loop in the  $z$  plane, parameterized by the angle  $\theta$ . The eigenvalues are

$$\lambda_{\pm}(\theta) = \pm i\sqrt{z(\theta)}. \quad (2.2)$$

The origin  $z = 0$ , for which  $H$  is a Jordan normal form, corresponds to the degeneracy on which our attention will focus. (The limit  $z \rightarrow \infty$  also corresponds to a Jordan form, but in the analysis to follow we will not need to emphasize this ‘degeneracy at infinity’.)

The time variable will also be  $\theta$ , representing cycles that are traversed uniformly. Therefore, states

$$|\psi(\theta)\rangle = \begin{Bmatrix} \psi_1(\theta) \\ \psi_2(\theta) \end{Bmatrix} \quad (2.3)$$

evolve according to the Schrödinger equation

$$i\partial_{\theta} |\psi(\theta)\rangle = H(\theta) |\psi(\theta)\rangle. \quad (2.4)$$

A scaling argument (appendix A) shows that slow cycling—the adiabatic case—corresponds, for this Hamiltonian, to loops far from the degeneracy at  $z = 0$ .

In later sections, we will compare the states evolving according to (2.4) with the instantaneous eigenstates of the operator  $H(\theta)$ , in which  $\theta$  is treated as a fixed parameter. In appendix B, we show that these must take the form

$$|ad_{\pm}(\theta)\rangle = |u_{\pm}(\theta)\rangle \exp\left\{-i \int_{\theta_0}^{\theta} d\theta' \lambda_{\pm}(\theta')\right\} = |u_{\pm}(\theta)\rangle \exp\{\mp i\gamma(\theta)\}, \quad (2.5)$$

in which the dynamical factor involves the exponent integrals

$$\gamma(\theta) = i \int_{\theta_0}^{\theta} d\theta' \sqrt{z(\theta')}, \quad (2.6)$$

$\theta_0$  is a constant, corresponding to an overall  $\theta$ -independent factor multiplying the state, and the vectors  $|u_{\pm}(\theta)\rangle$  are

$$|u_{\pm}(\theta)\rangle = \begin{Bmatrix} z(\theta)^{-1/4} \\ \pm z(\theta)^{+1/4} \end{Bmatrix}. \quad (2.7)$$

The branch-point at  $z = 0$  implies that around a loop that encloses the degeneracy the two eigenvalues (2.2) have exchanged, and so (up to a constant factor) have the eigenvectors (2.5)–(2.7) (the ‘flip’ [6]).

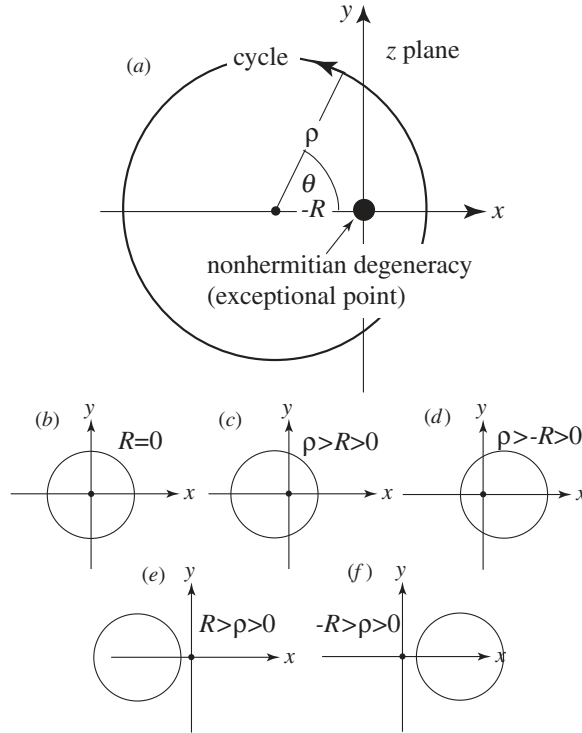
Before making the adiabatic connection with the instantaneous eigenstates, we will study exact solutions of the evolution equation (2.4). This can be written in terms of the individual components of the state vector:

$$\partial_{\theta}^2 \psi_1(\theta) = z(\theta) \psi_1(\theta), \quad \psi_2(\theta) = \partial_{\theta} \psi_1(\theta). \quad (2.8)$$

Thus, exactly solvable second-order ordinary differential equations can potentially represent loops for which the evolution (2.4) is exactly solvable. An example is polygonal loops, whose segments generate solutions in terms of Airy functions. It would be interesting to explore them further, but here we will concentrate on a different class of exact solutions.

We remark that since  $H(\theta)$  in (2.1) is traceless, Liouville’s formula ([27], pp 134–5) implies that the evolution operator  $K(\theta)$ , defined by

$$|\psi(\theta)\rangle = K(\theta) |\psi(0)\rangle, \quad (2.9)$$



**Figure 1.** Geometry of loop and degeneracy. (a) Notation; (b) degeneracy-centred loop (sections 5 and 6); (c) and (d) degeneracy-enclosing loops (section 7); (e) and (f) degeneracy-excluding loops (section 8).

which we will calculate explicitly in section 4, satisfies

$$\det [K(\theta)] = K_{11}(\theta)K_{22}(\theta) - K_{12}(\theta)K_{21}(\theta) = 1. \tag{2.10}$$

A consequence, which can also be derived using (2.4), is the following conservation law for any two evolving states  $|\psi_A(\theta)\rangle, |\psi_B(\theta)\rangle$ :

$$\psi_{A1}(\theta)\psi_{B2}(\theta) - \psi_{A2}(\theta)\psi_{B1}(\theta) = \text{constant}. \tag{2.11}$$

### 3. Excentric circular loops: exact solution and Floquet states

We choose

$$z(\theta) = \rho \exp(i\theta) - R, \tag{3.1}$$

corresponding (figure 1(a)) to a circular loop with radius  $\rho$ . The degeneracy, which lies at the origin of the  $z$  plane, is offset by  $R$  (positive or negative) from the centre of the loop.  $\rho > |R|$  corresponds to loops that enclose the degeneracy, and  $\rho < |R|$  to loops that exclude it. Figures 1(b)–(f) illustrate the different cases, to be considered in more detail in later sections.

The exact solutions of (2.8) can be written in terms of Bessel functions. From formula (10.13.6) of [28], there follow the solutions

$$|\psi(\theta)\rangle = \begin{Bmatrix} C_\nu(\zeta(\theta)) \\ \partial_\theta C_\nu(\zeta(\theta)) \end{Bmatrix} = \begin{Bmatrix} C_\nu(\zeta(\theta)) \\ \frac{1}{2}i[-\zeta(\theta)C_{\nu+1}(\zeta(\theta)) + \nu C_\nu(\zeta(\theta))] \end{Bmatrix}, \tag{3.2}$$

in which  $C_\nu$  represents any of

$$J_\nu(\zeta(\theta)), \quad J_{-\nu}(\zeta(\theta)), \quad Y_\nu(\zeta(\theta)), \quad Y_{-\nu}(\zeta(\theta)), \quad H_\nu^{(1)}(\zeta(\theta)), \quad H_\nu^{(2)}(\zeta(\theta)), \quad (3.3)$$

with order and argument

$$\nu = 2\sqrt{R}, \quad \zeta(\theta) = 2\sqrt{\rho} \exp\left(\frac{1}{2}i\theta\right). \quad (3.4)$$

At the beginning of the cycle ( $\theta = 0$ ), the argument  $\zeta$  is positive real, at the end ( $\theta = 2\pi$ ) it is negative real, and during the cycle it is complex. The order of the Bessel functions is real for positive offsets  $R$ , and purely imaginary for  $R < 0$ . We do not consider the more general case of complex  $R$ , in which the centre of the loop, as seen from the degeneracy, lies in an arbitrary direction. Nevertheless, the exact formulas above apply for arbitrary complex  $\nu$ .

Among the solutions, the two Floquet states are fundamental. These are the states that return to their original form after the cycle, apart from a complex factor. Continuation formulas for Bessel functions ((10.11.1) of [28]) enable these to be identified as

$$|F_\pm(\theta)\rangle = \begin{Bmatrix} J_{\pm\nu}(\zeta(\theta)) \\ \partial_\theta J_{\pm\nu}(\zeta(\theta)) \end{Bmatrix}, \quad (3.5)$$

with continuations

$$|F_\pm(2\pi)\rangle = \exp(\pm i\nu\pi)|F_\pm(0)\rangle. \quad (3.6)$$

Thus, for positive offsets ( $\nu$  real) the Floquet eigenvalues are pure phase factors, and for negative offsets ( $\nu$  imaginary) they are purely real exponentials.

The Floquet states are biorthogonal eigenvectors of the (nonunitary) cycle evolution operator: the left eigenvectors (row vectors which are the eigenvectors of the transposed cycle evolution operator) are

$$\langle F_\pm(\theta)| = \{\partial_\theta J_{\mp\nu}(\zeta(\theta)) - J_{\mp\nu}(\zeta(\theta))\}, \quad (3.7)$$

so

$$\langle F_\mp(\theta) | F_\pm(\theta)\rangle = 0. \quad (3.8)$$

The corresponding biorthogonal normalization,

$$\langle F_+(\theta) | F_+(\theta)\rangle = -\langle F_-(\theta) | F_-(\theta)\rangle = \frac{1}{2}i\zeta(J_\nu J'_{-\nu} - J_{-\nu} J'_\nu) = -i\frac{\sin(\nu\pi)}{\pi}, \quad (3.9)$$

follows from the Bessel Wronskian relation ((10.5.1) of [28]).

It is clear from (3.6) that the Floquet states are degenerate whenever  $\nu$  is an integer  $n$ , that is, for positive offsets

$$R = \frac{1}{4}n^2. \quad (3.10)$$

Then (3.9) shows that the two states  $|F_\pm(\theta)\rangle$  are self-orthogonal as well as biorthogonal. This degeneracy of the Floquet states is a degeneracy of the evolution operator, and should be distinguished from the unrelated degeneracy of the instantaneous eigenstates at  $z(\theta) = 0$ . More generally, the formal expressions for the exact evolving states (3.2) give no immediate indication of whether the loop encloses the degeneracy at  $z = 0$ . We will see that this distinction is an adiabatically asymptotic emergent phenomenon, associated with the different behaviour of the Bessel functions when their order is less than or greater than their argument.

#### 4. Exact solutions from adiabatic initial conditions

Alternative to the Floquet states are the states that start in each of the instantaneous eigenstates, namely

$$|\psi_{\pm}(0)\rangle = |ad_{\pm}(0)\rangle. \quad (4.1)$$

As measures of how closely the evolving states continue to cling to the instantaneous eigenstates, we define the adiabatic multipliers  $a_{\pm}(\theta)$ ,  $b_{\pm}(\theta)$  in

$$\begin{aligned} |\psi_{+}(\theta)\rangle &= a_{+}(\theta) |ad_{+}(\theta)\rangle + b_{+}(\theta) |ad_{-}(\theta)\rangle \\ |\psi_{-}(\theta)\rangle &= a_{-}(\theta) |ad_{+}(\theta)\rangle + b_{-}(\theta) |ad_{-}(\theta)\rangle. \end{aligned} \quad (4.2)$$

The multipliers can be calculated using biorthogonality. We define the adiabatic left eigenvectors as the instantaneous row eigenvectors corresponding to the transpose operator  $H^T(\theta)$ , namely

$$\langle ad_{\pm}(\theta)| = A_{\pm}(\theta) \langle u_{\pm}(\theta)|, \quad (4.3)$$

where

$$\langle u_{\pm}(\theta)| = \{\mp z(\theta)^{+1/4} - z(\theta)^{-1/4}\}, \quad (4.4)$$

and  $A_{\pm}(\theta)$  are arbitrary scalar functions that will cancel from the adiabatic multipliers. Then

$$\begin{aligned} a_{+}(\theta) &= \frac{\langle ad_{+}(\theta) | \psi_{+}(\theta) \rangle}{\langle ad_{+}(\theta) | ad_{+}(\theta) \rangle}, & b_{+}(\theta) &= \frac{\langle ad_{-}(\theta) | \psi_{+}(\theta) \rangle}{\langle ad_{-}(\theta) | ad_{-}(\theta) \rangle}, \\ a_{-}(\theta) &= \frac{\langle ad_{+}(\theta) | \psi_{-}(\theta) \rangle}{\langle ad_{+}(\theta) | ad_{+}(\theta) \rangle}, & b_{-}(\theta) &= \frac{\langle ad_{-}(\theta) | \psi_{-}(\theta) \rangle}{\langle ad_{-}(\theta) | ad_{-}(\theta) \rangle}. \end{aligned} \quad (4.5)$$

Obviously, these satisfy the initial conditions corresponding to (4.1):

$$\begin{aligned} a_{+}(0) &= 1, & b_{+}(0) &= 0 \\ a_{-}(0) &= 0, & b_{-}(0) &= 1. \end{aligned} \quad (4.6)$$

We can calculate the multipliers, in particular their values at the end of the cycle ( $\theta = 2\pi$ ), from the evolution operator  $K(\theta)$ , defined by (2.9), applied to the states we are interested in, defined by (4.1), that is,

$$|\psi_{\pm}(\theta)\rangle = K(\theta) |ad_{\pm}(0)\rangle. \quad (4.7)$$

To find  $K(\theta)$ , we write any exact evolving state as a superposition of Floquet states with constant coefficients, namely

$$|\psi(\theta)\rangle = \alpha |F_{+}(\theta)\rangle + \beta |F_{-}(\theta)\rangle, \quad (4.8)$$

with the constant coefficients determined by applying the biorthogonality relations (3.7)–(3.9) at  $\theta = 0$ . Thus,

$$\alpha = \frac{\langle F_{+}(0) | \psi(0) \rangle}{\langle F_{+}(0) | F_{+}(0) \rangle}, \quad \beta = \frac{\langle F_{-}(0) | \psi(0) \rangle}{\langle F_{-}(0) | F_{-}(0) \rangle}, \quad (4.9)$$

giving

$$K(\theta) = \frac{|F_{+}(\theta)\rangle \langle F_{+}(0)|}{\langle F_{+}(0) | F_{+}(0) \rangle} + \frac{|F_{-}(\theta)\rangle \langle F_{-}(0)|}{\langle F_{-}(0) | F_{-}(0) \rangle}. \quad (4.10)$$

To write explicit formulas for the multipliers at the end of the cycle, we use the Floquet continuations (3.6). Thus,

$$K(2\pi) = \exp(i\pi\nu) \frac{|F_{+}(0)\rangle \langle F_{+}(0)|}{\langle F_{+}(0) | F_{+}(0) \rangle} + \exp(-i\pi\nu) \frac{|F_{-}(0)\rangle \langle F_{-}(0)|}{\langle F_{-}(0) | F_{-}(0) \rangle}. \quad (4.11)$$

Then, with the abbreviations

$$\zeta = \zeta(0) = 2\sqrt{\rho}, \quad \nu = 2\sqrt{R}, \quad J_{\pm\nu} = J_{\pm\nu}(\zeta), \quad J'_{\pm\nu} = \partial_{\zeta} J_{\pm\nu}(\zeta), \quad (4.12)$$

a short calculation gives the matrix form for the evolution operator as

$$K(2\pi) = \begin{pmatrix} D - iA & B \\ C & D + iA \end{pmatrix}, \quad (4.13)$$

where

$$\begin{aligned} A &= \frac{1}{2}\pi\zeta (J_{\nu}J_{-\nu})', & B &= 2\pi J_{\nu}J_{-\nu}, \\ C &= \frac{1}{2}\pi\zeta^2 J'_{\nu}J'_{-\nu}, & D &= \cos(\pi\nu). \end{aligned} \quad (4.14)$$

These expressions are valid for all  $\nu$ , including  $\nu$  integer for which the Floquet states are degenerate. (These formulas confirm that  $K$  satisfies the Liouville relation (2.10).)

Finally, using formulas (2.7) and (4.4) for the vectors  $|u_{\pm}(\theta)\rangle$ ,  $\langle u_{\pm}(\theta)|$ , from which

$$\langle u_{\pm}(\theta) | u_{\mp}(\theta) \rangle = 0, \quad \langle u_{\pm}(\theta) | u_{\pm}(\theta) \rangle = \pm 2, \quad (4.15)$$

and using (2.5), we obtain the multipliers (4.5) in the following convenient form:

$$\begin{aligned} a_{+}(2\pi) &= -\frac{1}{2} \langle u_{+}(2\pi) | K(2\pi) | u_{+}(0) \rangle \exp \{i(\gamma(2\pi) - \gamma(0))\} \\ b_{+}(2\pi) &= \frac{1}{2} \langle u_{-}(2\pi) | K(2\pi) | u_{+}(0) \rangle \exp \{-i(\gamma(0) + \gamma(2\pi))\} \\ a_{-}(2\pi) &= -\frac{1}{2} \langle u_{+}(2\pi) | K(2\pi) | u_{-}(0) \rangle \exp \{i(\gamma(0) + \gamma(2\pi))\} \\ b_{-}(2\pi) &= \frac{1}{2} \langle u_{-}(2\pi) | K(2\pi) | u_{-}(0) \rangle \exp \{i(\gamma(0) - \gamma(2\pi))\}. \end{aligned} \quad (4.16)$$

A consequence of the analogous relations for general  $\theta$ , together with (2.7) and the Liouville formula (2.10), is the following conservation law, for any loop, circular or not and degeneracy-enclosing or not:

$$a_{+}(\theta)b_{-}(\theta) - a_{-}(\theta)b_{+}(\theta) = \det [K(\theta)] = 1. \quad (4.17)$$

A word about normalization. It is obvious from (4.5) that the multipliers are independent of the normalization of the left eigenvectors ( $A_{\pm}(\theta)$  in (4.3)). And the exponential factors in (4.16) show that the multipliers  $a_{+}$  and  $b_{-}$ , that is, the ones with initial values unity (cf (4.6)), are independent of the constant  $\theta_0$  in the exponent (2.6). But the multipliers  $a_{-}$  and  $b_{+}$ , that is, the ones with initial values zero, representing the initially unoccupied states, are not independent of  $\theta_0$ . Alternatively stated, if in definitions (2.5)  $|ad_{+}(\theta)\rangle$  is multiplied by  $C_{+}$  and  $|ad_{-}(\theta)\rangle$  by  $C_{-}$ , this leaves  $a_{+}$  and  $b_{-}$  unchanged, but changes  $b_{+}$  by  $C_{+}/C_{-}$  and  $a_{-}$  by  $C_{-}/C_{+}$ . This underdetermination also occurs in the Hermitian case, where it is commonly eliminated (up to phase) by the convention of normalizing the instantaneous eigenstates by the Hermitian conjugate—a procedure that would be artificial here, where the dynamical factors accompanying the eigenstates vary in modulus as well as phase and there seems to be no natural normalization. In each of the cases to follow (corresponding to figures 1(b)–(f)), we will state the form of  $\gamma(\theta)$  that is being used.

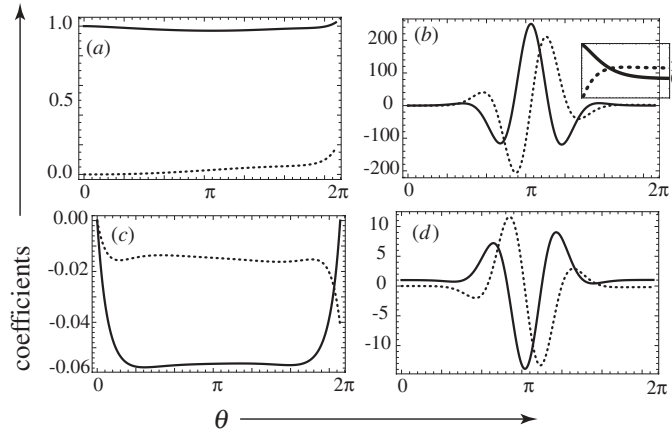
### 5. Degeneracy-centred loop

This is  $R = 0$  (figure 1(b)). From (3.1) and (2.5)–(2.7), we can choose

$$\gamma(\theta) = 2\sqrt{\rho} \exp\left(\frac{1}{2}i\theta\right) = \zeta(\theta), \quad (5.1)$$

so the adiabatic states are

$$|ad_{\pm}(\theta)\rangle = \left\{ \begin{array}{l} \exp\left(-\frac{1}{4}i\theta\right) \rho^{-1/4} \\ \pm \exp\left(\frac{1}{4}i\theta\right) \rho^{+1/4} \end{array} \right\} \exp\{\mp i\gamma(\theta)\}. \quad (5.2)$$



**Figure 2.** Adiabatic multipliers for  $R = 0$ ,  $\rho = 4.2$  (section 5), for (a)  $a_+(\theta)$ ; (b)  $b_+(\theta)$ ; (c)  $a_-(\theta)$ ; (d)  $b_-(\theta)$ . Full curves: real part; dotted curves: imaginary part. Note the very different values of the multipliers. The inset in (b) shows the final value of  $b_+(\theta)$ , close to  $2i$ .

At the beginning and end of the cycle, the instantaneous eigenstates are related by (cf (4.12))

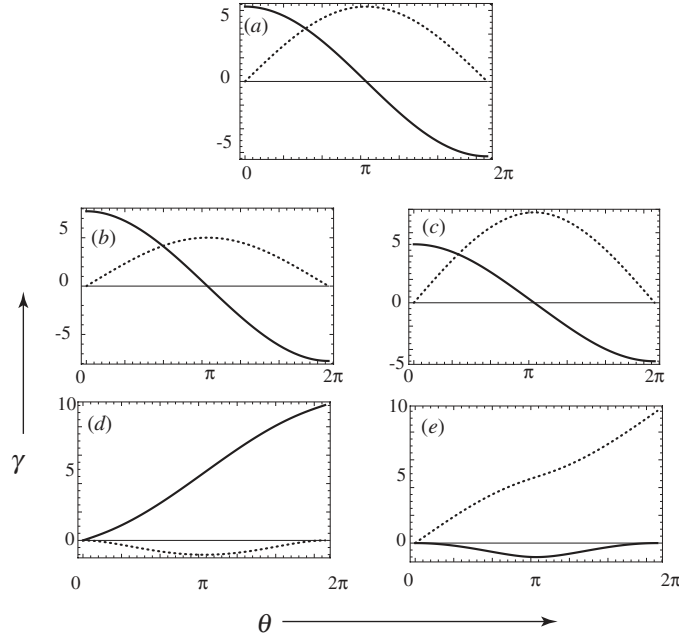
$$|ad_{\pm}(0)\rangle = \begin{pmatrix} \rho^{-1/4} \\ \pm \rho^{+1/4} \end{pmatrix} \exp(\mp i\zeta), \quad |ad_{\pm}(2\pi)\rangle = -i |ad_{\mp}(0)\rangle. \quad (5.3)$$

The second equation exemplifies the flip [6] associated with loops enclosing the degeneracy. Its coefficient  $-i$  represents the geometric phase, with the state returning exactly only after four cycles; the sign change after two cycles corresponds to that around a diaboloical point of a Hermitian operator, which can be regarded as two coincident degeneracies of a non-Hermitian operator.

Figure 2 shows the evolution of the corresponding adiabatic multipliers, as computed either from (4.5) with the states  $|\psi_{\pm}(\theta)\rangle$  computed numerically from the Schrödinger equation (2.4), or analytically using the evolution operator (4.10). As expected on the adiabatic assumption that the evolving states cling close to the instantaneous eigenvectors, the multiplier  $a_+(\theta)$  of the initially occupied eigenvector in the state  $|\psi_+(\theta)\rangle$  remains close to unity, and the multiplier  $a_-(\theta)$  of the initially unoccupied eigenvector in the state  $|\psi_-(\theta)\rangle$  remains close to zero. But the multiplier  $b_+(\theta)$  of the initially unoccupied eigenvector in the state  $|\psi_+(\theta)\rangle$  does not remain close to zero as expected. Instead, it fluctuates enormously, and settles down to a final value, at  $\theta = 2\pi$ , close to  $2i$  (inset in figure 2(b)). And although the final value of the multiplier  $b_-(\theta)$  of the initially occupied eigenvector in the state  $|\psi_-(\theta)\rangle$  is close to the expected value unity, there are large fluctuations during the cycle.

As a first step in explaining these phenomena, consider figure 3(a), which shows  $\text{Re } \gamma$  and  $\text{Im } \gamma$  (equation (5.1)). Because  $\text{Im } \gamma > 0$  during the cycle, the eigenstate  $|ad_+(\theta)\rangle$  in (5.2) is exponentially dominant over  $|ad_-(\theta)\rangle$ . Now, the Stokes phenomenon of asymptotics [11, 12] is the change in multipliers of exponentially small contributions to a function when masked by exponentially large ones. This explains why the multiplier  $b_+$  can vary during the cycling of the state  $|\psi_+(\theta)\rangle$ . In the state  $|\psi_-(\theta)\rangle$ , the corresponding subdominant multiplier  $b_-$  also fluctuates, but less strongly than  $b_+$  because the eigenstate  $|ad_+(\theta)\rangle$  that would dominate it is largely unoccupied, so the masking is weaker.





**Figure 3.**  $\text{Re } \gamma(\theta)$  (full curves) and  $\text{Im } \gamma(\theta)$  (dotted curves) for (a) degeneracy-centred loop  $\rho = 10, R = 0$ ; excentric degeneracy-enclosing loops (b)  $\rho = 10, R = 4.3$ , (c)  $\rho = 10, R = -4.3$ ; excentric degeneracy-excluding loops (d)  $\rho = 1.5, R = 2.3$ , (e)  $\rho = 1.5, R = -2.3$ .

At the end of the cycle, the exact multipliers are given by (4.16), in which the evolution operator  $K(2\pi)$  in (4.13) simplifies because orders of the Bessel functions in (4.14) are zero or unity. A short calculation gives

$$\begin{aligned} a_+(2\pi) &= [b_-(2\pi)]^* = \frac{1}{2}i\pi\zeta \exp(-2i\zeta) (J_0 + iJ_1)^2 \\ b_+(2\pi) &= \frac{1}{2}i(2 + \pi\zeta(J_0^2 + J_1^2)) \\ a_-(2\pi) &= \frac{1}{2}i(2 - \pi\zeta(J_0^2 + J_1^2)). \end{aligned} \tag{5.4}$$

Adiabatically, that is for large cycles, the Bessel functions can be approximated by their large-argument asymptotic forms ((10.17.3) of [28]), leading to

$$a_+(2\pi) \rightarrow 1, \quad b_+(2\pi) = 2i, \quad a_-(2\pi) \rightarrow 0, \quad b_-(2\pi) \rightarrow 1. \tag{5.5}$$

Of these final multipliers,  $a_+, a_-$  and  $b_-$  conform to the naive adiabatic expectation that slowly-cycled evolving states will return to the instantaneous eigenstates at the end of the cycle. But  $b_+$  does not; again this is an example of the Stokes phenomenon, with the subdominant multiplier having changed irrevocably. As Stokes himself put it [29] (reprinted in [30]),

‘... the inferior term enters as it were into mist, is hidden for a little from view, and comes out with its coefficient changed...’.

In the next section, we examine this in more detail.

### 6. Superadiabatic approximations for degeneracy-centred loops

One might expect that the exact evolving states will cling more closely to approximate states that include higher order (superadiabatic [19, 20]) corrections to the instantaneous

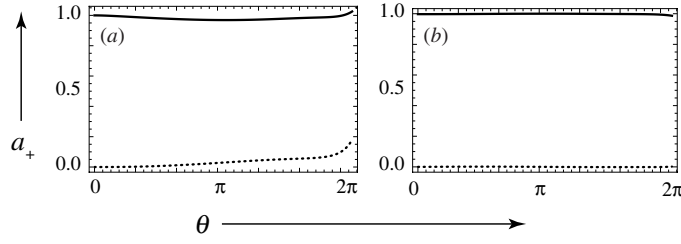


Figure 4. As figure 2, for superadiabatic coefficients (section 6)  $a_+(\theta)$ . (a)  $n = 0$ ; (b)  $n = 1$ .

eigenstates. For degeneracy-centred cycles, we can find these corrections by observing that the eigenstates (5.2) involve the lowest-order large-argument approximations to the Hankel functions  $H_0^{(1)}$ ,  $H_0^{(2)}$  and their derivatives, and these functions are exact solutions of the Schrödinger equation (cf (3.2) and (3.3)). This enables  $n$ th-order approximations to the evolving states to be identified from known asymptotic expansions of the Hankel functions (e.g. (10.17.5), (10.17.6), (10.17.11) and (10.17.12) of [28], or (8.451.3) and (8.451.4) of [31]). These superadiabatic approximations are

$$\begin{aligned}
 |ad_+(n, \theta)\rangle &= \left\{ \begin{array}{l} \exp(-\frac{1}{4}i\theta) \rho^{-1/4} \sum_{k=0}^n \frac{c_k}{(2i\zeta(\theta))^k} \\ \exp(\frac{1}{4}i\theta) \rho^{+1/4} \sum_{k=0}^n \frac{d_k}{(2i\zeta(\theta))^k} \end{array} \right\} \exp\{-i\zeta(\theta)\} \\
 |ad_-(n, \theta)\rangle &= \left\{ \begin{array}{l} \exp(-\frac{1}{4}i\theta) \rho^{-1/4} \sum_{k=0}^n \frac{(-1)^k c_k}{(2i\zeta(\theta))^k} \\ -\exp(\frac{1}{4}i\theta) \rho^{+1/4} \sum_{k=0}^n \frac{(-1)^k d_k}{(2i\zeta(\theta))^k} \end{array} \right\} \exp\{i\zeta(\theta)\},
 \end{aligned}
 \tag{6.1}$$

where the coefficients are

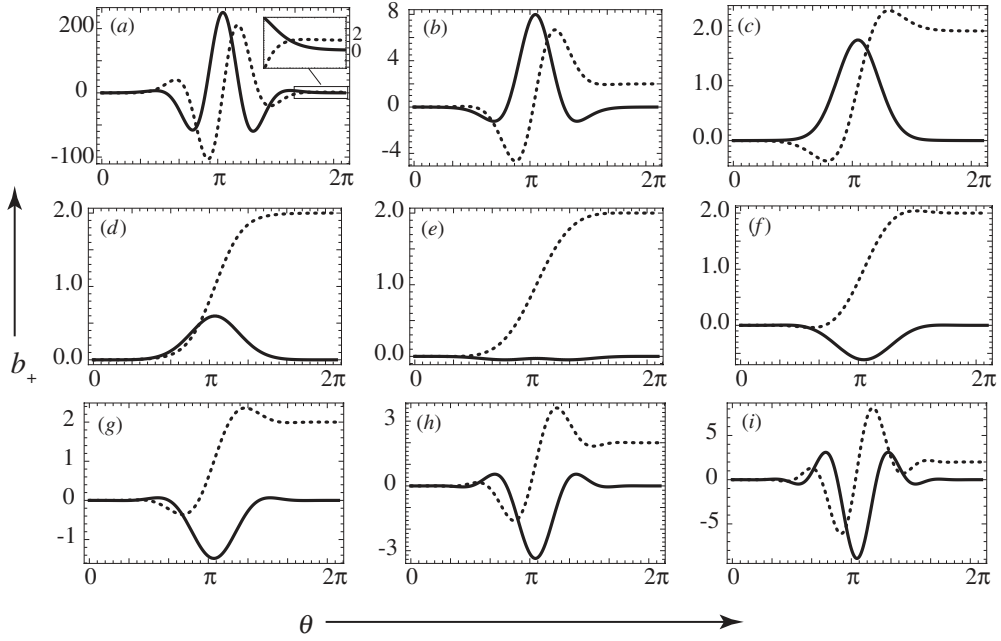
$$c_k = \frac{\Gamma(k + \frac{1}{2})}{k! \Gamma(-k + \frac{1}{2})}, \quad d_k = \frac{\Gamma(k + \frac{3}{2})}{k! \Gamma(-k + \frac{3}{2})}.
 \tag{6.2}$$

(This corresponds to the adiabatic perturbation series method of [20], rather than the iterative renormalization method used in [19].)

The corresponding superadiabatic multipliers are defined by analogy with (4.5), with  $|ad_+(n, \theta)\rangle$  replacing  $|ad_+(\theta)\rangle$ , etc, and can easily be computed numerically. Figure 4 illustrates how for the multiplier  $a_+(\theta)$  even the first superadiabatic correction substantially improves the clinging to the exact evolving state.

Figure 5 shows the most interesting case, of the multiplier  $b_+(\theta)$  for increasing superadiabatic orders  $n$ . For all  $n$ , this multiplier changes from its initial value, 0, to its final value, close to  $2i$  (cf (5.5)). But the manner of the change depends dramatically on  $n$ : the fluctuations reduce rapidly as  $n$  increases, up to an optimal value ( $n = 8$  in the example in figure 5(e)), after which they start to grow again.

This behaviour is an example of a common asymptotic phenomenon [21, 22]: across a Stokes line, at which one exponential maximally dominates another, the subdominant multiplier, when the dominant asymptotic series is truncated near its least term (‘optimal truncation’), increases rapidly but smoothly, according to an error function. A brief summary of how the theory works in the present case is given in appendix C. Maximal domination occurs



**Figure 5.** As figure 4, for  $b_+(\theta)$ . (a)–(i)  $n = \{0, 2, 4, \dots, 16\}$ . Note how the increase of the coefficients from 0 to  $2i$  (in (a) shown as inset) gets smoother as the optimal order  $n = 8$  (figure (e)) is approached, and fluctuates again thereafter.

at  $\theta = \pi$  (cf figure 3(a)), where the difference of the exponents of the two exponentials—the ‘singulant’ [10]—is purely real. The singulant is

$$\sigma(\rho, \theta) = -2i\zeta(\theta) = -4i\sqrt{\rho} \exp\left(\frac{1}{2}i\theta\right). \tag{6.3}$$

For  $\theta$  near  $\pi$ , where  $\sigma(\rho, \pi) = 4\sqrt{\rho}$ , optimal truncation occurs near

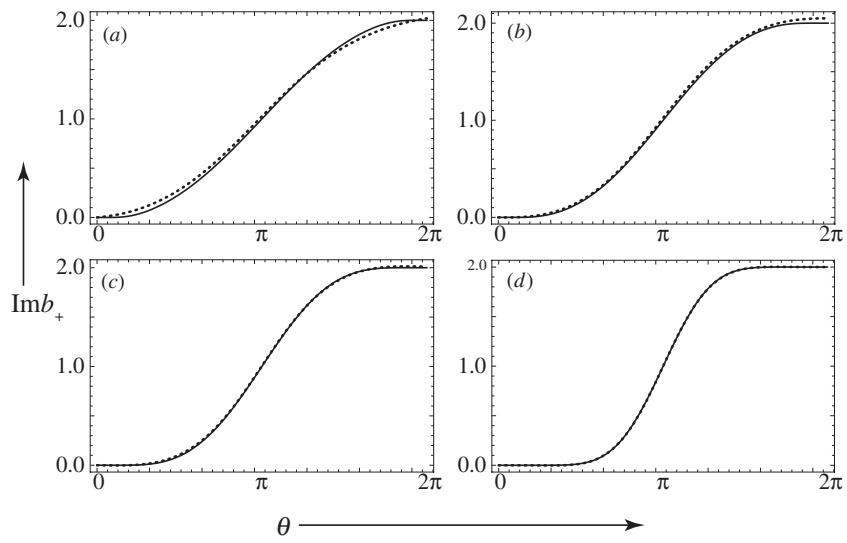
$$n^* = \text{int}(4\sqrt{\rho}), \tag{6.4}$$

(for figure 5(e),  $n^* = 8$ ). At this order, the general theory gives the multiplier

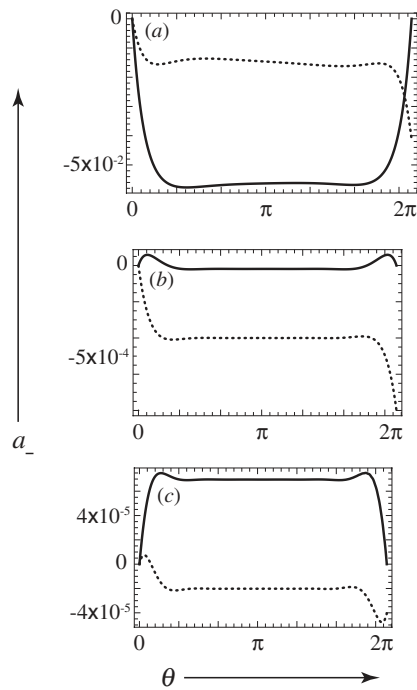
$$b_{+\text{optimal}}(\theta) = i \operatorname{erfc}\left(-\frac{\operatorname{Im} \sigma(\rho, \theta)}{\sqrt{2\operatorname{Re} \sigma(\rho, \theta)}}\right). \tag{6.5}$$

As figure 6 shows, this asymptotic theory describes evolution of the multiplier very accurately, even for small values of  $\rho$ . The only slightly non-standard feature of the present example is that the ‘Stokes constant’, giving the multiplier after the Stokes line has been crossed, is  $2i$  rather than  $i$  as in elementary examples [21, 32]; this reflects the well-understood Stokes constants associated with Bessel’s equation [11] for  $\nu = 0$ , and we will encounter it again in the next section in the more general context of excentric cycles. (For non-standard Stokes constants in Hermitian evolution, see [33].)

For the remaining multipliers  $a_-$  and  $b_-$ , corresponding to the evolving state  $|\psi_-(\theta)\rangle$ , no Stokes phenomenon is expected, because the dominant eigenstate is initially unoccupied. And indeed figures 7 and 8 show that increasing  $n$  makes these multipliers keep more closely to their initial values—that is, the superadiabatic approximations cling more closely to the exact evolving state.



**Figure 6.** Comparison of exact optimally-truncated superadiabatic  $b_+(\theta)$  coefficients (dotted curves) with universal Stokes-line-crossing error-function approximation (6.5) (smooth curves), for (a)  $\rho = 1/4$  (optimal order  $n = 2$ ); (b)  $\rho = 1/2$  (optimal order  $n = 3$ ); (c)  $\rho = 1$  (optimal order  $n = 4$ ); (d)  $\rho = 4$  (optimal order  $n = 8$ ).



**Figure 7.** As figure 4, for  $a_-(\theta)$ . (a)–(c)  $n = \{0, 3, 6\}$ .

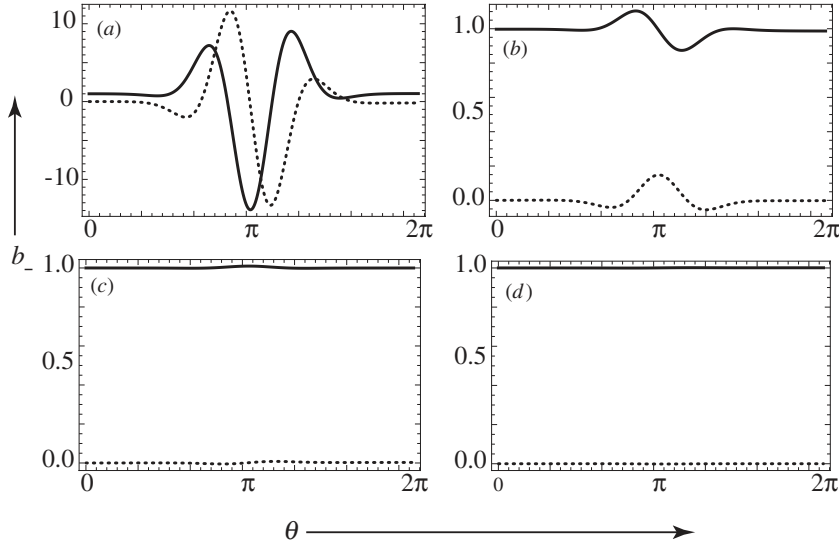


Figure 8. As figure 4, for  $b_-(\theta)$ . (a)–(d)  $n = \{0, 1, 2, 3\}$ .

### 7. Excentric degeneracy-enclosing loops

Loops enclose the degeneracy excentrically if  $\rho > |R| > 0$  (figures 1(c) and (d)). To avoid phase ambiguity, it is convenient to write the fourth roots in the instantaneous eigenstates (2.5) and (2.7) as

$$z(\theta)^{1/4} = \exp\left(\frac{1}{4}i\theta\right) (\rho - R \exp(-i\theta))^{1/4}. \tag{7.1}$$

Similarly, the integrals (2.6) in the dynamical factors can be written

$$\gamma(\theta) = 2 \left[ \sqrt{\rho - R \exp(-i\theta)} \exp\left(\frac{1}{2}i\theta\right) - \sqrt{R} \cos^{-1}\left(\exp\left(-\frac{1}{2}i\theta\right) \sqrt{\frac{R}{\rho}}\right) + \frac{1}{2}\pi\sqrt{R} \right]. \tag{7.2}$$

With this implicit choice of  $\theta_0$ ,  $\gamma(\theta)$  is real at the beginning and end of the cycle and antisymmetric about  $\theta = \pi$ , as illustrated in figures 3(b) and (c), with explicit forms conveniently written separately for  $R > 0$  and  $R < 0$  as

$$\begin{aligned} \gamma(0) &= -\gamma(2\pi) \\ &= \left. \begin{aligned} &2 \left[ \sqrt{\rho - R} - \sqrt{R} \cos^{-1}\left(\sqrt{\frac{R}{\rho}}\right) + \frac{1}{2}\pi\sqrt{R} \right] & (R > 0) \\ &2 \left[ \sqrt{\rho + |R|} - \sqrt{|R|} \sinh^{-1}\left(\sqrt{\frac{|R|}{\rho}}\right) \right] & (R < 0) \end{aligned} \right\} \end{aligned} \tag{7.3}$$

(the derivations use  $\cos^{-1}(ix) = \frac{1}{2}\pi - i \sinh^{-1}x$  and  $\cos^{-1}(-x) = \pi - \cos^{-1}x$ ).

These ingredients enable the explicit calculation of the final multipliers (4.16). After some reduction, the result is

$$\begin{aligned}
 a_+(2\pi) &= [b_-(2\pi)]^* = \frac{1}{2}i\pi \exp(-2i\gamma_0) \left( -i\zeta (J_\nu J_{-\nu})' + \sqrt{\zeta^2 - \nu^2} J_\nu J_{-\nu} - \frac{\zeta^2 J'_\nu J'_{-\nu}}{\sqrt{\zeta^2 - \nu^2}} \right) \\
 b_+(2\pi) &= \frac{1}{2}i \left( 2 \cos \nu\pi + \pi \sqrt{\zeta^2 - \nu^2} J_\nu J_{-\nu} + \pi \frac{\zeta^2 J'_\nu J'_{-\nu}}{\sqrt{\zeta^2 - \nu^2}} \right) \\
 a_-(2\pi) &= \frac{1}{2}i \left( 2 \cos \nu\pi - \pi \sqrt{\zeta^2 - \nu^2} J_\nu J_{-\nu} - \pi \frac{\zeta^2 J'_\nu J'_{-\nu}}{\sqrt{\zeta^2 - \nu^2}} \right).
 \end{aligned} \tag{7.4}$$

These exact formulas satisfy

$$\begin{aligned}
 b_+(2\pi) + a_-(2\pi) &= 2i \cos \nu\pi \\
 a_+(2\pi)b_-(2\pi) - a_-(2\pi)b_+(2\pi) &= 1.
 \end{aligned} \tag{7.5}$$

The first equation is obvious, and the second is a special case of the conservation law (4.17).

To establish the adiabatic asymptotic forms of these multipliers, it is convenient to consider offsets  $R > 0$  (i.e.  $\nu$  real) and  $R < 0$  (i.e.  $\nu$  imaginary) separately.

### 7.1. $\rho > R > 0$ (figure 1(c))

In this case, the order of the Bessel functions is real, and we eliminate the negative orders using

$$J_{-\nu}(\zeta) = J_\nu(\zeta) \cos \nu\pi - Y_\nu(\zeta) \sin \nu\pi. \tag{7.6}$$

Then use of standard Debye asymptotics (large order, argument  $>$  order, see (10.19.6) and (10.19.7) of [28]) in lowest approximation, leads to

$$\begin{aligned}
 a_+(2\pi) &\rightarrow 1, & b_+(2\pi) &= 2i \cos \nu\pi = 2i \cos(2\pi\sqrt{R}), \\
 a_-(2\pi) &\rightarrow 0, & b_-(2\pi) &\rightarrow 1.
 \end{aligned} \tag{7.7}$$

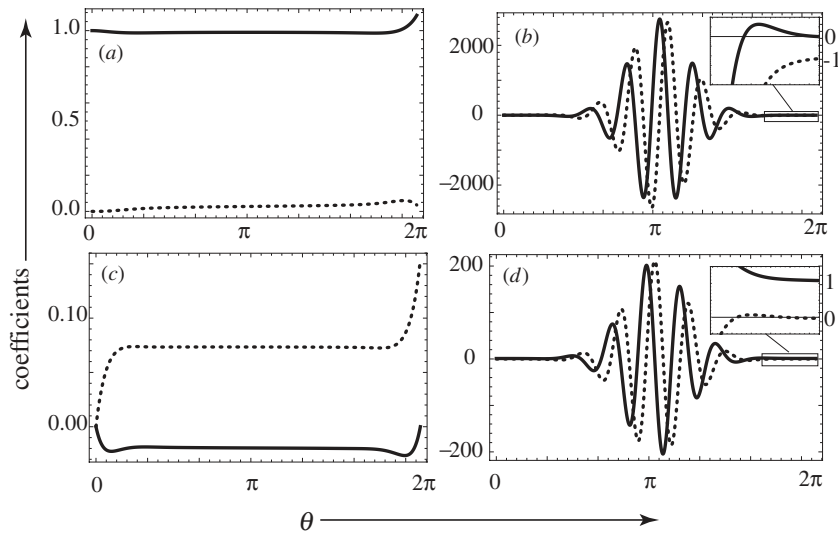
This is similar to the behaviour (5.5) for degeneracy-centred cycles, except that the asymptotic form  $b_+(2\pi)$  is  $2i \cos \nu\pi$  rather than  $2i$ , reflecting the Stokes constants associated with the Bessel equation for arbitrary order [34]. An interesting special class is offsets  $R = \frac{1}{16}(2n+1)^2$ , for which the Bessel order  $\nu$  is half-integer. Then,  $b_+(2\pi)$  is zero, that is, the initially unoccupied state is again unoccupied at the end of the cycle. This happens because Bessel functions of half-integer order are represented exactly in terms of trigonometric functions (sections 10.47 and 10.49 of [28]): the asymptotic series terminates, so there is no divergence and no Stokes phenomenon.

Figure 9 shows the evolution of the multipliers, for a case where the Stokes constant is  $i$ . The behaviour is similar to that for degeneracy-centred cycles (cf figure 2). And figure 10 shows the final multipliers for increasing adiabaticity, that is, as  $\rho$  increases with  $\rho/R$  fixed, in good agreement with the asymptotic forms (7.7). Note in particular figure 10(b), which shows the variation with the Stokes multiplier  $\cos(2\pi\sqrt{R})$ , in dramatic contradiction of the naive intuition that for slow cycling the initially unoccupied state would remain so.

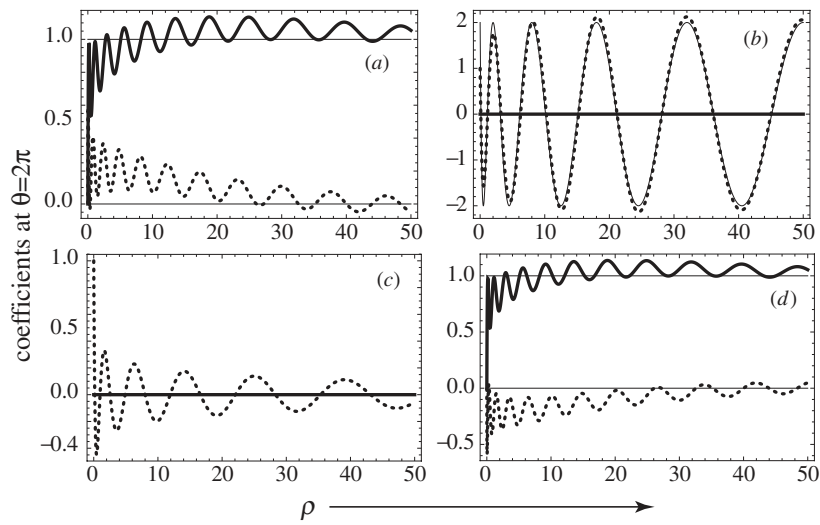
### 7.2. $\rho > -R > 0$ (figure 1(d))

To find the adiabatic approximations to the final multipliers (7.4) in this case, it is convenient to connect Bessel functions of positive and negative imaginary order and real argument using

$$J_{i|\nu|}(\zeta) = [J_{-i|\nu|}(\zeta)]^*. \tag{7.8}$$



**Figure 9.** As figure 2, for excentric degeneracy-enclosing cycle  $\rho = 15$ ,  $R = 64/9$ . Inset for (b) shows approach to the predicted coefficient (cf (7.7)  $b_+(2\pi) = 2i \cos(\pi 2\sqrt{64/9}) = -i$ ); inset for (d) shows approach to the predicted coefficient  $b_-(2\pi) = 1$ .



**Figure 10.** Final coefficients for excentric degeneracy-enclosing loops  $R = \rho/2$ , for (a)  $a_+(2\pi)$ ; (b)  $b_+(2\pi)$ ; (c)  $a_-(2\pi)$ ; (d)  $b_-(2\pi)$  (full curves: real part; dotted curves: imaginary part), showing approach to adiabatic asymptotic values (7.7). Part (d) also illustrates the relation  $b_-(2\pi) = a_+(2\pi)^*$ .

The relevant large-order Bessel asymptotics is less familiar, and the lowest-order leading asymptotic expressions are insufficient. We need the formulas, which can be obtained from

results in [35],

$$J_{i|v|}(\zeta) = \frac{\exp\left\{i\left(\sqrt{|v|^2 + \zeta^2} - |v| \sinh^{-1}\left(\frac{|v|}{\zeta}\right) - \frac{1}{4}\pi\right) + \frac{1}{2}\pi|v|\right\}}{\sqrt{2\pi}(|v|^2 + \zeta^2)^{1/4}} \times \left(1 - i \frac{U_1(|v|/\sqrt{|v|^2 + \zeta^2})}{|v|} - \frac{U_2(|v|/\sqrt{|v|^2 + \zeta^2})}{|v|^2} + \dots\right) \quad (7.9)$$

and

$$J'_{i|v|}(\zeta) = \frac{\exp\left\{i\left(\sqrt{|v|^2 + \zeta^2} - |v| \sinh^{-1}\left(\frac{|v|}{\zeta}\right) + \frac{1}{4}\pi\right) + \frac{1}{2}\pi|v|\right\}}{\sqrt{2\pi}\zeta} \times (|v|^2 + \zeta^2)^{1/4} \left(1 - i \frac{V_1(|v|/\sqrt{|v|^2 + \zeta^2})}{|v|} - \frac{V_2(|v|/\sqrt{|v|^2 + \zeta^2})}{|v|^2} + \dots\right), \quad (7.10)$$

in which  $U_{1,2}(p)$  and  $V_{1,2}(p)$  are polynomials listed in (10.41.10) and (10.41.11) of [28].

Substitution of these approximations into (7.4) requires care, because although leading-order exponentials cancel, suggesting limiting multipliers  $a_+$  and  $a_-$  analogous to those in (7.7) for  $R > 0$ , corrections to these exponentials (requiring the polynomials  $U_{1,2}(p)$  and  $V_{1,2}(p)$ ) do not cancel and lead to uncompensated large exponentials. After some reduction, we obtain the leading-order asymptotic final multipliers

$$a_+(2\pi) = [b_-(2\pi)]^* \rightarrow -\frac{\rho \exp(2\pi\sqrt{|R|})}{8(\rho + |R|)^{3/2}} \times \exp\left(-4i \left[ \sqrt{\rho + |R|} - \sqrt{|R|} \sinh^{-1}\left(\sqrt{\frac{|R|}{\rho}}\right) \right]\right) \quad (7.11)$$

$$b_+(2\pi) \rightarrow 2i \cosh(2\pi\sqrt{|R|})$$

$$a_-(2\pi) \rightarrow -i \exp(2\pi\sqrt{|R|}) \frac{\rho^2}{64(\rho + |R|)^3}.$$

The result for  $b_+(2\pi)$  is the Stokes constant for the Bessel function of imaginary order  $2i\sqrt{|R|}$ .

Figure 11 illustrates the evolution of the multipliers for this case. The curves are very different from those for  $R \geq 0$ , with the enormous variations, again contradicting naive adiabatic intuition, arising from the large real exponentials in the Bessel functions of imaginary order, though the Stokes variation in the subdominant multipliers  $b_+$  and  $b_-$  is still evident. Figure 12 shows the final multipliers for increasing adiabaticity, that is as functions of  $\rho$  for fixed  $\rho/|R|$ . The large variations require logarithmic plots; the discrepancy between the exact and asymptotic multipliers is invisible over the range illustrated.

### 8. Excentric degeneracy-excluding loops

Loops do not enclose the degeneracy if  $|R| > \rho$  (figures 1(e) and (f)). Then there is no flip of the instantaneous eigenstates, because (with a convenient choice of phase)

$$z(\theta)^{1/4} = \left. \begin{array}{l} \exp\left(-\frac{1}{4}i\pi\right) (R - \rho \exp(i\theta))^{1/4} (R > 0) \\ (|R| + \rho \exp(i\theta))^{1/4} (R < 0) \end{array} \right\} \quad (8.1)$$

is singlevalued round the loop. An important limiting case, which we will concentrate on here, is  $\rho \ll |R|$ , that is, very small loops. For these, the eigenvectors and eigenvalues are



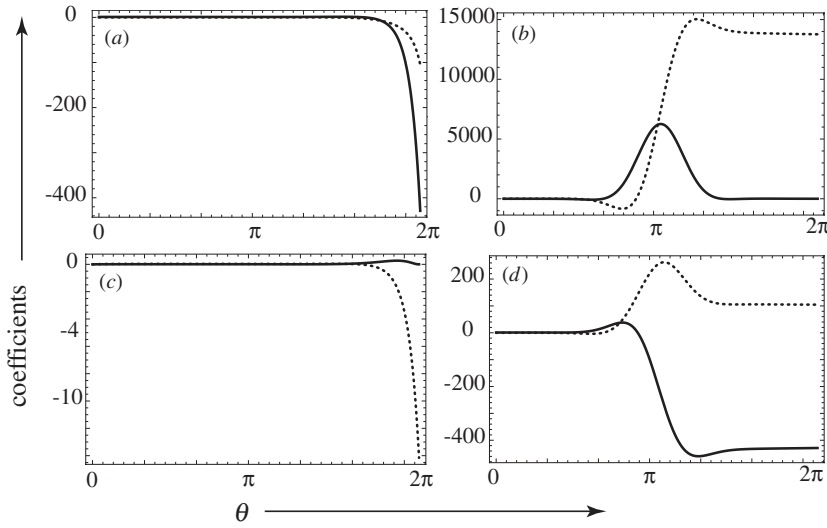


Figure 11. As figure 2, for excentric degeneracy-enclosing loop  $\rho = 4.2$ ,  $R = -2.3$ .

almost constant, so we expect the adiabatic multipliers to change very little during the cycle: no Stokes phenomenon and almost perfect clinging. In this section we will show how the limit follows from our general formulas. This might seem just a reassurance exercise, but we will see that the approach to the limit can be extremely slow. It will be convenient to give the explicit formulas for positive and negative offsets.

Convenient general forms for the exponent integrals (2.6), illustrated in figures 3(d) and (e) are

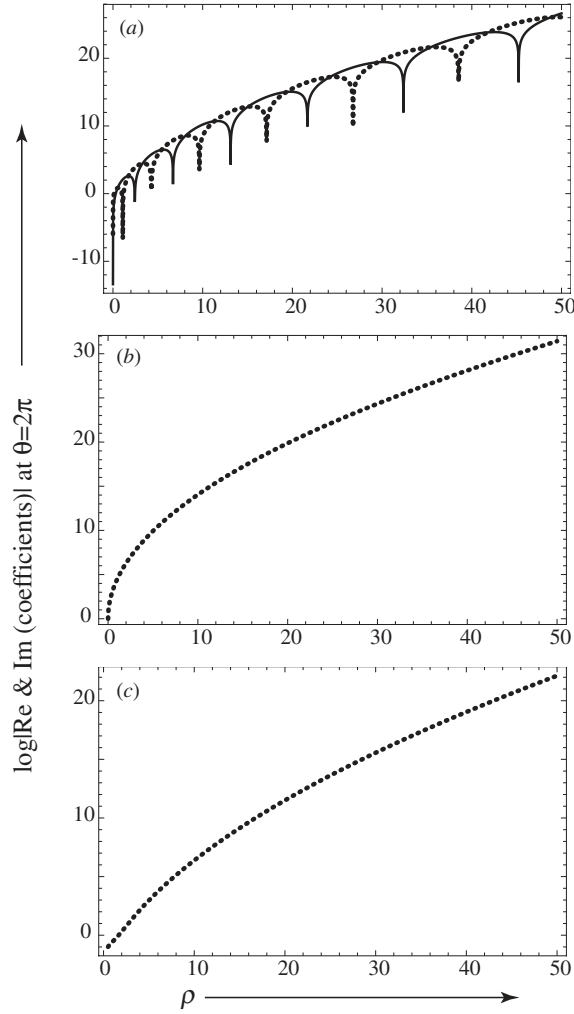
$$\gamma(\theta) = \left. \begin{aligned} & \theta\sqrt{R} - 2i \left[ \sqrt{R - \rho \exp(i\theta)} - \sqrt{R - \rho} \right. \\ & \left. - \sqrt{R} \log \left( \frac{\sqrt{R - \rho \exp(i\theta)} + \sqrt{R}}{\sqrt{R - \rho} + \sqrt{R}} \right) \right] \quad (R > \rho > 0) \\ & i\theta\sqrt{R} + 2 \left[ \sqrt{|R| + \rho \exp(i\theta)} - \sqrt{|R| + \rho} \right. \\ & \left. - \sqrt{|R|} \log \left( \frac{\sqrt{|R| + \rho \exp(i\theta)} + \sqrt{|R|}}{\sqrt{|R| + \rho} + \sqrt{|R|}} \right) \right] \quad (-R > \rho > 0). \end{aligned} \right\} \quad (8.2)$$

For  $\rho \ll |R|$ , approximate expressions are

$$\gamma(\theta) \approx \left. \begin{aligned} & \theta\sqrt{R} - \frac{\rho \sin \theta}{2\sqrt{R}} - i \frac{\rho}{\sqrt{R}} \sin^2 \frac{1}{2}\theta \quad (R \gg \rho > 0) \\ & i\theta\sqrt{|R|} + i \frac{\rho \sin \theta}{2\sqrt{|R|}} - \frac{\rho}{\sqrt{|R|}} \sin^2 \frac{1}{2}\theta \quad (-R \gg \rho > 0) \end{aligned} \right\}. \quad (8.3)$$

Thus, as  $\rho \rightarrow 0$ , the instantaneous eigenstates approach

$$\begin{aligned} |ad_{\pm}(\theta)\rangle &= \begin{pmatrix} \exp\left(\frac{1}{4}i\pi\right) R^{-1/4} \\ \exp\left(-\frac{1}{4}i\pi\right) R^{1/4} \end{pmatrix} \exp(\mp i\theta\sqrt{R}) \quad (R \gg \rho > 0) \\ |ad_{\pm}(\theta)\rangle &= \begin{pmatrix} |R|^{-1/4} \\ |R|^{1/4} \end{pmatrix} \exp(\pm\theta\sqrt{|R|}) \quad (-R \gg \rho > 0). \end{aligned} \quad (8.4)$$



**Figure 12.** Final coefficients for excentric degeneracy-enclosing loop  $R = -\rho/2$ , for (a)  $\log|\text{Re}(a_+(2\pi))|$  (full curve) and  $\log|\text{Im}(a_+(2\pi))|$  (dotted curve); (b)  $\log|\text{Im}(b_+(2\pi))|$ ; (c)  $\log|\text{Im}(a_-(2\pi))|$ ; the curves are indistinguishable from the adiabatic approximations (7.11). ( $b_- = (a_+)^*$  so we do not plot this multiplier.)

For positive offset, the dynamical factor acquires a pure phase during the evolution, and for negative offset there is gain for the + state and loss for the – state.

Calculation of the final multipliers from (4.16) requires the evolution operator given by (4.13) and (4.14). The limit  $\rho \rightarrow 0$  requires the small-argument limiting form of the Bessel functions ((10.7.3) of [28]). Using this, and the reflection formula for the gamma function, leads to

$$K(\theta) = \left. \begin{aligned} & \left( \begin{array}{cc} \cos(\theta\sqrt{R}) & \sin(\theta\sqrt{R})/\sqrt{R} \\ -\sin(\theta\sqrt{R})\sqrt{R} & \cos(\theta\sqrt{R}) \end{array} \right) (R \gg \rho > 0) \\ & \left( \begin{array}{cc} \cosh(\theta\sqrt{|R|}) & \sinh(\theta\sqrt{|R|})/\sqrt{|R|} \\ \sinh(\theta\sqrt{|R|})\sqrt{|R|} & \cosh(\theta\sqrt{|R|}) \end{array} \right) (-R \gg \rho > 0) \end{aligned} \right\}. \tag{8.5}$$

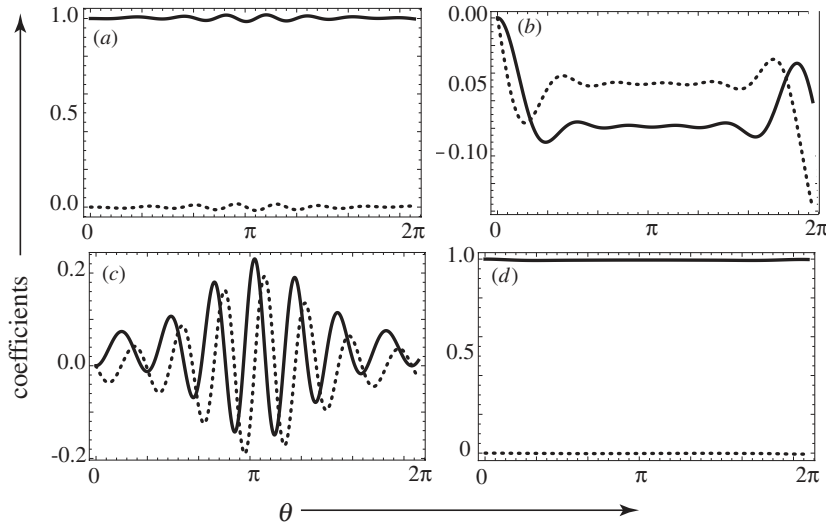


Figure 13. As figure 2, for excentric degeneracy-excluding loop  $\rho = 4.5$ ,  $R = 9.4$ .

With this formula, and (8.4), a calculation based on (4.16) confirms that the final adiabatic multipliers are exactly equal to their initial values (4.6):  $a_+(2\pi) = 1$ ,  $b_+(2\pi) = 0$ ,  $a_-(2\pi) = 0$ ,  $b_-(2\pi) = 1$ .

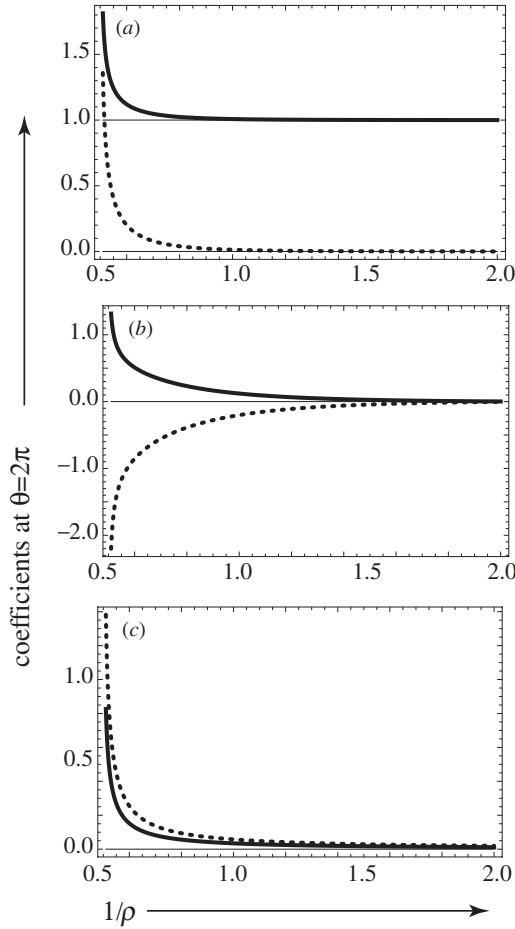
Figure 13 shows the evolution of the adiabatic multipliers for a degeneracy-excluding loop with positive offset  $R = 9.4$  and radius  $\rho = 4.5$ ; they remain fairly close to their initial values, even for these loops for which  $\rho$  is not very small. Figure 14 shows the rapid convergence of the final multipliers to these initial values as the loops get smaller.

For negative offset, the behaviour is less simple. Figure 15 shows the evolution of the multipliers for offset  $R = -2.4$  and radius  $\rho = 0.5$ .  $a_+(\theta)$  and  $a_-(\theta)$  cling close to the initial values as expected, but  $b_+(\theta)$  and  $b_-(\theta)$  veer dramatically away near the end of the cycle. This is because these are the multipliers of the exponentially small evolving instantaneous eigenstate (cf. (8.4)), so their contribution to each of the exact evolving states is masked by that of the exponentially dominant eigenstate. Because of this, and as figures 16(b) and (c) illustrate, convergence of the final multipliers  $b_+(2\pi)$  and  $b_-(2\pi)$  to the initial values is very slow, perhaps over scales  $\rho \sim \exp(4\pi \sqrt{|R|})$  (we have not pursued the asymptotics to the degree required to establish the precise convergence rate).

### 9. Transitionless non-Hermitian evolution

We have discussed the inevitable changes in the adiabatic multipliers—transitions between instantaneous eigenstates—for time-dependent Hamiltonians. But it is worth noting briefly that within the slightly different framework in which  $H(\theta)$  given by (2.1) is replaced by a different Hamiltonian  $\tilde{H}(\theta)$ , we can ensure that there are no transitions at all between the adiabatic states (2.5) of (2.1). This ‘transitionless driving’ (a kind of reverse engineering) is the subject of recent work [23–25] on Hermitian evolutions, which originated in a study of reflectionless potentials [36] and applies also in the non-Hermitian case [26]. To find the new Hamiltonian  $\tilde{H}(\theta)$ , we first write (2.1) in terms of the Pauli matrices, that is,

$$H(\theta) = i \begin{pmatrix} 0 & 1 \\ z(\theta) & 0 \end{pmatrix} = \mathbf{R}(\theta) \cdot \boldsymbol{\sigma}, \tag{9.1}$$



**Figure 14.** Final coefficients for excentric degeneracy-excluding loops with  $R = 2$ , showing convergence to asymptotic values—the same as initial values (4.6)—as the loop radius  $\rho$  gets smaller: (a)  $a_+(2\pi)$ ; (b)  $b_+(2\pi)$ ; (c)  $a_-(2\pi)$  (full curves: real part; dotted curves: imaginary part). ( $b_- = (a_+)^*$  so we do not plot this multiplier.)

where

$$\mathbf{R}(\theta) \cdot \boldsymbol{\sigma} = \frac{1}{2}(\mathbf{i}(1 + z(\theta))\sigma_x - (1 - z(\theta))\sigma_y). \tag{9.2}$$

Then we use result (3.8) of [25], to get

$$\begin{aligned} \tilde{H}(\theta) &= H(\theta) + \frac{\mathbf{R}(\theta) \times \mathbf{R}'(\theta) \cdot \boldsymbol{\sigma}}{2\mathbf{R}(\theta) \cdot \mathbf{R}(\theta)} \\ &= \mathbf{i} \begin{pmatrix} -\frac{\partial_\theta z(\theta)}{4z(\theta)} & 1 \\ z(\theta) & \frac{\partial_\theta z(\theta)}{4z(\theta)} \end{pmatrix} = \begin{pmatrix} \frac{(z(\theta)+R)}{4z(\theta)} & \mathbf{i} \\ \mathbf{i}z(\theta) & -\frac{(z(\theta)+R)}{4z(\theta)} \end{pmatrix}. \end{aligned} \tag{9.3}$$

The second equality applies to any Hamiltonian of the form (2.1), and the third applies to the special case (3.1) that we have concentrated on. It can be checked explicitly that under  $\tilde{H}(\theta)$  the exact evolving states are the adiabatic states (2.5), that is,

$$\mathbf{i}\partial_\theta |ad_\pm(\theta)\rangle = \tilde{H}(\theta) |ad_\pm(\theta)\rangle. \tag{9.4}$$

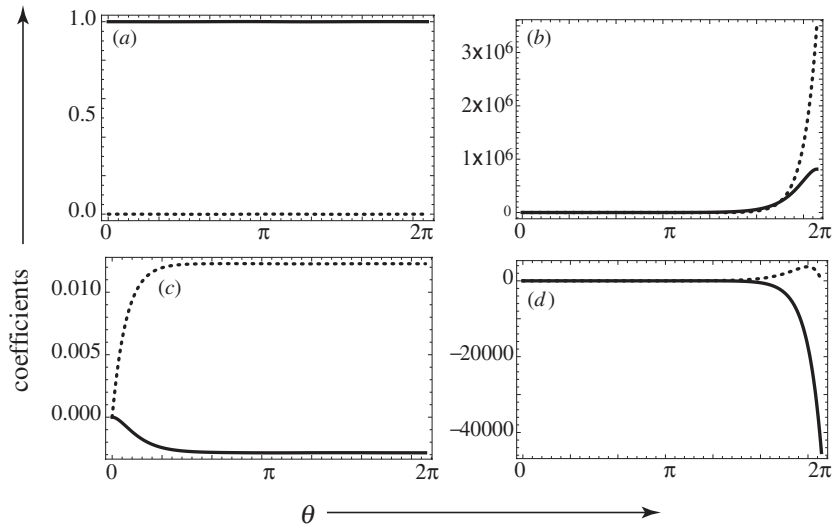


Figure 15. As figure 2, for excentric degneracy-excluding loop  $\rho = 0.5$ ,  $R = -2.4$ .

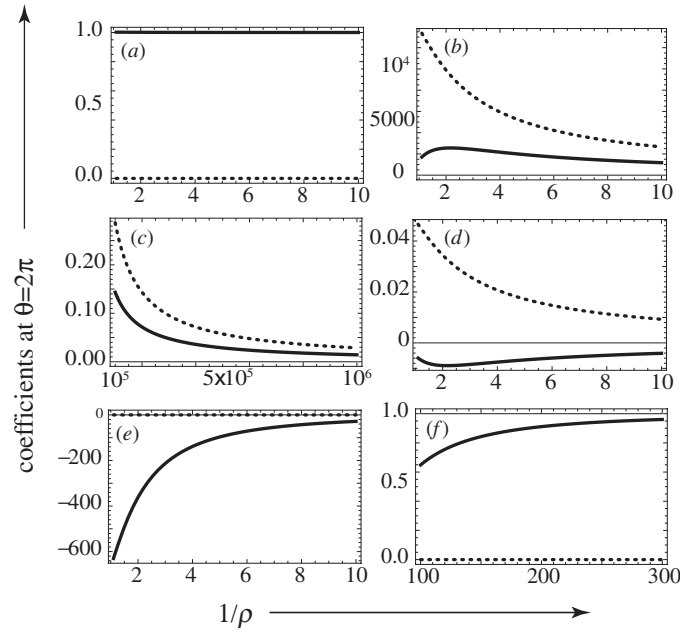


Figure 16. Final coefficients for excentric degneracy-excluding loops with  $R = -1$ , showing convergence to asymptotic values—the same as initial values (4.6)—as the loop radius  $\rho$  gets smaller: (a)  $a_+(2\pi)$ ; (b)  $b_+(2\pi)$ ; (c)  $b_+(2\pi)$  for smaller loops; (d)  $a_-(2\pi)$ ; (e)  $b_-(2\pi)$ ; (f)  $b_-(2\pi)$  for smaller loops (full curves: real part; dotted curves: imaginary part). The slow convergence is illustrated in (c) and (f).

This implies  $a_+(\theta) = 1$ ,  $b_+(\theta) = 0$ ,  $a_-(\theta) = 0$ ,  $b_-(\theta) = 1$  for all  $\theta$ . (Note that the behaviour of  $b_+(\theta)$ —constant for all  $R$  and  $\rho$  as well as  $\theta$ —is to be distinguished from that

for the special values of  $R$  discussed after (7.7), for which  $b_+$  is transitionless only the end of the cycle.)

This holds independently of any adiabatic approximation. But when the evolution is slow, the problem arises of why the Stokes asymptotics, associated with the degeneracy at  $z = 0$ , does not apply, particularly for  $b_+(\theta)$ —that is, why does  $\tilde{H}(\theta)$  suppress the transitions that occur for  $H(\theta)$ ? The reason (too complicated to go into in detail here but previously discussed in related contexts [25, 36]), is that the additional term in  $\tilde{H}(\theta)$  splits the degeneracy at  $z = 0$  into three, given by the solution of

$$-(\partial_\theta z)^2 = (R + z)^2 = 16z^3. \quad (9.5)$$

For transitionless Hamiltonians, the combined effect of the cluster of degeneracies is to make the asymptotic series terminate, so there is no divergence and no Stokes phenomenon. Another way to see this is to note that the second-order differential equation satisfied by  $\psi_1$  (after eliminating  $\psi_2$ ) is satisfied by Bessel functions of half-integer order (cf the remarks in the paragraph following (7.7)).

## 10. Concluding remarks

The analysis reported here has explored, with the aid of an exactly solvable model, the occupancies (adiabatic multipliers) of the instantaneous eigenstates of evolving vectors as they are driven round a loop in the space of parameters of a non-Hermitian Hamiltonian. As was noted before [6], some of the multipliers behave very differently from those driven by a Hermitian Hamiltonian: even in the adiabatic regime of slow cycling, these multipliers can vary enormously, violating naive adiabatic intuition. We have shown how these variations exemplify the Stokes phenomenon of asymptotics, and the exactly solvable model has the advantage that precise explicit formulas to be obtained using known properties of Bessel functions.

But the study presented here is far from complete, and we now list some directions for future work. We described the Floquet solutions and also the solutions that start in instantaneous eigenstates (and, in section 6, in superadiabatically corrected states). But there at least two alternative evolutions which deserve further study and which we have begun to explore. First are the ‘periodic modes’ [6], in which the adiabatic multipliers return to their original values, up to a constant. And second, there are the evolutions of states whose asymptotics are pure exponentials to all orders; for degeneracy-enclosing loops with positive offset, these are the states (3.2) involving the Bessel functions  $H_\nu^{(1,2)}(\zeta)$  (this option is only possible for exactly solvable models).

For degeneracy-excluding loops (section 8), our analysis was restricted to very small loops. For larger loops, precise description of the exponentially large variations on the multipliers, while not involving flip, requires delicate control of the Bessel asymptotics. We have made some progress in this direction but results are not definitive.

The offsets we have considered are those in which  $R$  is positive real or negative real, for which the eigenvalues at the beginning and end of the loop are purely real or purely imaginary. The more general possibility is complex  $R$ , for which the centre of the loop is offset from the degeneracy in an arbitrary direction, corresponding to initial and final eigenvalues that are complex. Studying these would require asymptotics of Bessel functions of arbitrary complex order (and of course complex argument), not just purely real as for real positive offset or purely imaginary as for real negative offset. One result would be that the Stokes constant  $2i \cos(\pi\nu)$  giving the large  $R$  asymptotic value of the coefficient  $b_+(2\pi)$  can take any complex value.

As mentioned in section 2, there are different exactly solvable cycles, corresponding to Schrödinger equations (2.8) representing exactly solvable one-dimensional quantum potentials. As well as polygonal loops for which the solutions involve the Airy function, these include loops around one or two degeneracies, involving confluent hypergeometric functions. It would be helpful to have a systematic classification.

Finally, we suggest that a promising area in which the evolutions studied here could be explored experimentally is the paraxial optics of space-varying crystals or liquid crystals. In a spatially uniform material that is biaxially anisotropic and both chiral and absorbing, the operator governing the evolution of light fields is a direction-dependent degenerate nonsymmetric  $2 \times 2$  matrix derived from Maxwell's equations [37, 38]. For certain propagation directions ('singular axes'), the matrix is degenerate, and sufficiently close to a singular axis the matrix has the form studied here [13]. When such a material, with a singular axis slightly inclined relative to the direction of a propagating light wave, is twisted through a complete turn, the evolution of the wave is paraxial if the twist is gentle (i.e. adiabatic). The cycled operator that governs the evolution depends on the medium's local singular axis, turning relative to the propagation direction. The adiabatic multipliers we have studied correspond to the changing distribution of the light between the two local polarization states (instantaneous eigenstates of the propagation matrix). This idea has been elaborated very recently [39] in a detailed study of the evolving polarization state of the light during such a degeneracy-enclosing cycle.

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### Appendix A. Adiabatic scaling

The time-dependent Schrödinger equation, for a cycle over time  $T$  round a loop in the  $Z$  plane, can be written

$$i\hbar\partial_t \begin{pmatrix} \phi_1(t) \\ \phi_2(t) \end{pmatrix} = i \begin{pmatrix} 0 & E_0 \\ Z\left(\frac{2\pi}{T}t\right) & 0 \end{pmatrix} \begin{pmatrix} \phi_1(t) \\ \phi_2(t) \end{pmatrix}, \quad (\text{A.1})$$

in which  $E_0$  is an energy parameter. With the (non-standard) scaling

$$\begin{aligned} \frac{2\pi}{T}t = \theta, \quad Z\left(\frac{2\pi}{T}t\right) &= \frac{1}{E_0} \left(\frac{\hbar}{T}\right)^2 z(\theta), \\ \begin{pmatrix} \phi_1(t) \\ \phi_2(t) \end{pmatrix} &= \begin{pmatrix} \sqrt{\frac{TE_0}{\hbar}} \psi_1(\theta) \\ \sqrt{\frac{\hbar}{TE_0}} \psi_2(\theta) \end{pmatrix}, \end{aligned} \quad (\text{A.2})$$

this becomes (2.1). Then the exact solutions (3.2) become

$$|\psi(t)\rangle = \begin{Bmatrix} D \\ \partial_t D \end{Bmatrix}, \quad (\text{A.3})$$

where

$$D = C_{\frac{1}{2}\sqrt{R}} \left( \frac{2}{\omega} \sqrt{\rho} \exp\left(\frac{1}{2}i\omega t\right) \right), \quad \omega = \frac{2\pi}{T}, \quad (\text{A.4})$$

and  $C_v$  is given by (3.3).

The adiabatic regime (slow cycling) corresponds to large  $T$  with the loop  $Z(\theta)$  fixed, and therefore to large  $z(\theta)$ , that is, according to (A.2), large loops in (2.1), as claimed. In the

solutions (A.4), large  $T$  corresponds to Bessel functions whose order and argument are both large, except for centred loops, for which the order is zero.

### Appendix B. Right and wrong adiabatic solutions

This is a nonrigorous argument justifying (2.4). The instantaneous eigenstates of  $H(\theta)$  satisfy

$$H(\theta) |ad_{\pm}(\theta)\rangle = \pm i\sqrt{z(\theta)} |ad_{\pm}(\theta)\rangle. \quad (\text{B.1})$$

This eigenequation leaves the eigenstates undetermined by a scalar factor which can depend on  $\theta$ . This must be fixed (up to a  $\theta$ -independent constant of course) by requiring that the adiabatic states satisfy the evolution equation (2.4) to lowest order.

Substituting (B.1) into (2.4), we must have

$$\partial_{\theta} |ad_{\pm}(\theta)\rangle \approx \begin{pmatrix} 0 & 1 \\ z(\theta) & 0 \end{pmatrix} |ad_{\pm}(\theta)\rangle = \pm\sqrt{z(\theta)} |ad_{\pm}(\theta)\rangle. \quad (\text{B.2})$$

The adiabatic approximation of ignoring transitions between the  $+$  and  $-$  states requires projection onto the adiabatic subspace to which each solution is restricted. We do this by introducing the biorthogonal bra vectors  $\langle ad_{\pm}(\theta)|$ , giving

$$\langle ad_{\pm}(\theta)| \partial_{\theta} |ad_{\pm}(\theta)\rangle \approx \pm\sqrt{z(\theta)} \langle ad_{\pm}(\theta)| ad_{\pm}(\theta)\rangle. \quad (\text{B.3})$$

Obviously, this implies that the dynamical factor involving  $\gamma(\theta)$  defined in (2.7) must be incorporated, in order to eliminate the  $\pm\sqrt{z(\theta)}$  term. But this is not enough: for if we substitute

$$|ad_{\pm}(\theta)\rangle = \exp\left(\pm \int^{\theta} d\theta' \sqrt{z(\theta')}\right) |u_{\pm}(\theta)\rangle \quad (\text{B.4})$$

into (B.3), we get that the vectors  $|u_{\pm}(\theta)\rangle$ , as well as being instantaneous eigenstates of  $H(\theta)$ , must also satisfy

$$\langle u_{\pm}(\theta)| \partial_{\theta} |u_{\pm}(\theta)\rangle = 0, \quad (\text{B.5})$$

that is, they must be parallel-transported.

An example of a pair of vectors that does not satisfy this condition is

$$|u_{1,\pm}(\theta)\rangle = \begin{pmatrix} 1 \\ \pm\sqrt{z(\theta)} \end{pmatrix}, \quad (\text{B.6})$$

because

$$\begin{aligned} \langle u_{1,\pm}(\theta)| \partial_{\theta} |u_{1,\pm}(\theta)\rangle &= (\mp\sqrt{z(\theta)} - 1)\partial_{\theta} \left( \frac{1}{\pm\sqrt{z(\theta)}} \right) \\ &= \mp \frac{\partial_{\theta} z(\theta)}{\sqrt{z(\theta)}} \neq 0. \end{aligned} \quad (\text{B.7})$$

By contrast, (2.7) does satisfy (B.5), as is easily checked:

$$\begin{aligned} \langle u_{\pm}(\theta)| \partial_{\theta} |u_{\pm}(\theta)\rangle &= \\ (\mp(z(\theta))^{+1/4} - (z(\theta))^{-1/4})\partial_{\theta} \begin{pmatrix} (z(\theta))^{-1/4} \\ \pm (z(\theta))^{+1/4} \end{pmatrix} &= 0. \end{aligned} \quad (\text{B.8})$$

Ignoring condition (B.5) would correspond, in Hermitian quantum mechanics, to ignoring the geometric phase. Forgetting this in the non-Hermitian situation would be more serious, because the error would not correspond simply to a phase.



### Appendix C. Stokes smoothing for degeneracy-centred solution

It will suffice to consider just the series in (6.1) with the coefficients  $c_k$  defined in (6.2). As a function of  $\theta$ , the series with upper limits  $n$  are truncations of the formal infinite series

$$S(\theta) = \sum_{k=0}^{\infty} \frac{c_k}{(2i\zeta(\theta))^k}, \quad (\text{C.1})$$

in which  $\zeta(\theta)$  is defined in (3.4). Successive application of the reflection formula and an asymptotic relation for the gamma function ((5.5.3) and (5.11.12) of [28]) give the high-order coefficients as

$$c_k = \frac{\Gamma(k + \frac{1}{2})}{k! \Gamma(-k + \frac{1}{2})} = (-1)^k \frac{\Gamma(k + \frac{1}{2})^2}{\pi k!} \approx (-1)^k \frac{(k-1)!}{\pi}. \quad (\text{C.2})$$

Thus, the series  $S(\theta)$  can be separated into a ‘head’, in which the exact form of the coefficients is retained, and a ‘tail’, in which the approximation is used:

$$S(\theta) \approx \sum_{k=0}^N \frac{c_k}{(2i\zeta(\theta))^k} + \frac{1}{\pi \sigma(\rho, \theta)} \sum_{k=N}^{\infty} \frac{k!}{\sigma(\rho, \theta)^k}, \quad (\text{C.3})$$

where  $\sigma(\rho, \theta)$  is the singulant (6.3). The series diverges: from Stirling’s formula ((5.11.3) of [28]), the terms get smaller and then increase, with the minimum near  $k = n^*$  defined by (6.4). As recognized by Stokes himself [40], the divergence is most severe on the Stokes line, because when  $\sigma$  is real and positive, all terms in the series have the same sign. For truncation near the least term, that is  $N \approx n^*$ , a variant of Borel summation ([21], see also [41]) enables the tail to be summed, with the result

$$\frac{1}{\pi \sigma(\rho, \theta)} \sum_{\text{int}(F(\theta) + \frac{1}{2})}^{\infty} \frac{k!}{\sigma(\rho, \theta)^k} \approx \frac{2i}{\sqrt{\pi}} \int_{-\infty}^{\frac{\text{Im}\sigma(\rho, \theta)}{2\sqrt{\text{Re}\sigma(\rho, \theta)}}} dt \exp(-t^2), \quad (\text{C.4})$$

from which (6.5) follows.

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