Discrete Phase Integral Method for Five-Term Recursion Relations

Anupam Garg*
Department of Physics and Astronomy, Northwestern University, Evanston, Illinois 60208
(October 24, 2018)

Abstract

A formalism is developed to study certain five-term recursion relations by discrete phase integral (or Wentzel-Kramers-Brillouin) methods. Such recursion relations arise naturally in the study of the Schrödinger equation for certain spin Hamiltonians. The conditions for the validity of the phase integral approximation are derived. It is shown that in contrast to the three-term problem, it is now possible to get a turning points “under the barrier”, i.e., in the classically forbidden region, as well as inside the classically allowed region. Further, no qualitatively new types of turning points arise in recursion relations with still higher numbers of terms. The phase integral approximation breaks down at the new turning points, requiring new connection formulas, which are derived.

75.10Dg, 03.65.Sq, 36.90+f, 75.45.+j
I. INTRODUCTION

The purpose of this paper is to develop the formalism of the discrete phase integral (DPI), or Wentzel-Kramers-Brillouin method, for cases where the recursion relation involves five terms. Previous use of this method has, as far as we are aware, been limited to three-term recursion relations [1–5]. Surprisingly, the extension to five terms is not routine, and entails novel physical and mathematical considerations. Further, once this extension is understood, no additional concepts are required in dealing with recursion relations involving still more terms.

The physical problem which led the author to consider this extension concerns the magnetic molecular cluster [(tacn)$_6$Fe$_8$O$_2$(OH)$_{12}$]$^{8+}$ (or just Fe$_8$ for short). This molecule has a total spin $J = 10$ in its ground state, and crystallizes into a solid where the cluster has an approximate $D_2$ symmetry. The interaction between molecules is very weak, and the low temperature spin dynamics of a single molecule are well described by the Hamiltonian

$$\mathcal{H} = -k_2 J_z^2 + (k_1 - k_2) J_x^2 - g \mu_B \mathbf{J} \cdot \mathbf{H}. \quad (1.1)$$

Here, $\mathbf{J}$ is a dimensionless spin operator, $\mathbf{H}$ is an externally applied magnetic field, and $k_1 > k_2 > 0$. (Experiments reveal $k_1 \approx 0.33$ K, and $k_2 \approx 0.22$ K.)

The spectrum of the Hamiltonian (1.1) shows some extremely interesting features as a function of the applied field $\mathbf{H}$. In particular, one finds a large number of diabolical points in the $H_x$-$H_z$ plane [10–12], which have also been seen experimentally [13]. Exactly as in the spectrum of a particle confined to a triangular box [9], some of the diabolical points (those arising when $\mathbf{H} \parallel \hat{x}$ or $\mathbf{H} \parallel \hat{z}$) can be related to a geometrical symmetry [14], but others cannot.

The problem was first studied [10] by instanton methods when $\mathbf{H} \parallel \hat{x}$, but this method is much harder to apply for general field orientations, and the phase integral method proves to be simpler. The existence of diabolical points turns out to depend critically on having five terms in the recursion relation that we shall describe shortly, and three terms would never lead to such points. The calculations which pertain specifically to Fe$_8$ are described elsewhere [15], but it seems worthwhile to present the formal aspects of the work separately, as they are more generally applicable.

A. Heuristic discussion of the DPI approximation

It is useful to continue with the above example in order to introduce the DPI method. The starting point of the procedure is to write Schrödinger’s equation in the $J_z$ basis. Let $\mathcal{H}|\psi\rangle = E|\psi\rangle$, $J_z|m\rangle = m|m\rangle$, $\langle m|\psi\rangle = C_m$, and $\langle m|\mathcal{H}|m'\rangle = t_{m,m'}$. Then,

$$\sum_{n=m-2}^{m+2} t_{m,n} C_n = E C_m. \quad (1.2)$$

The diagonal terms ($t_{m,m}$) in the above equation arise from the $J_z^2$ and $J_z H_z$ parts of $\mathcal{H}$, those off-diagonal by one ($t_{m,m+1}$) from the $J_x H_z$ and $J_y H_y$ parts, and those off-diagonal by two ($t_{m,m+\pm2}$) from the $J_x^2$ part.

The DPI method is applicable to a recursion relation such as (1.2) whenever the $t_{m,m+\alpha}$ ($\alpha = 0, 1, 2$) vary sufficiently slowly with $m$. A physical analogy may be made with an
electron hopping on a lattice with on-site energies $t_{m,m}$ and nearest-neighbor and next-nearest-neighbor hopping terms $t_{m,m\pm 1}$ and $t_{m,m\pm 2}$. If these quantities were independent of $m$, the solutions to Eq. (1.2) would be Bloch waves $C_m = \exp(\imath q m)$, with an energy

$$E = w_m + 2t_{m,m+1}\cos q + 2t_{m,m+2}\cos 2q \equiv E(q),$$

(1.3)

where we have written $w_m \equiv t_{m,m}$ to highlight the physically different role of the on-site energy from the hopping terms. We shall use the notations $w_m$ and $t_{m,m}$ interchangeably. If for fixed $\alpha$, the $t_{m,m+\alpha}$ vary slowly with $m$ (where the meaning of this term remains to be made precise), we expect it to be a good approximation to introduce a local Bloch wavevector, $q(m)$, and write $C_m$ as an exponential $e^{\imath \Phi}$, whose phase $\Phi$ accumulates approximately as the integral of $q(m)$ with increasing $m$, in exactly the same way that in the continuum quasiclassical method in one dimension, one writes the wavefunction as $\exp(\imath S(x)/\hbar)$, and approximates $S(x)$ as the integral of the local momentum $p(x)$.

It is obvious that the above approximation will entail the replacement of various sums by integrals, and to that end, we introduce smooth functions $t_\alpha(m)$ of a continuous variable $m$ as extensions of $t_{m,m+\alpha}$ such that whenever $m$ is an integer

$$t_\alpha(m) = (t_{m,m+\alpha} + t_{m,m-\alpha})/2, \quad \alpha = 0, 1, 2.$$  \hfill (1.4)

We will try and choose these functions so that their derivatives are small. The precise way in which this is to be done will be discussed later, but supposing that we have been successful in finding such functions, we can seek to approximate $C_m$ in exact parallel with the continuum phase integral approach. The form of the solution that emerges, and which readers will readily appreciate from knowledge of the continuum case, is given by

$$C_m \sim \frac{1}{\sqrt{v(m)}} \exp \left( \imath \int^m q(m') dm' \right),$$  \hfill (1.5)

where $q(m)$ and $v(m)$ obey the equations

$$E = w(m) + 2t_1(m)\cos q + 2t_2(m)\cos 2q \equiv \mathcal{H}_{sc}(q, m),$$  \hfill (1.6)

$$v(m) = \partial \mathcal{H}_{sc}/\partial q = -2\sin q(m)(t_1(m) + 4t_2(m)\cos q(m)).$$  \hfill (1.7)

[Just as for the matrix elements, we define $w(m) \equiv t_0(m)$, and use the notation $w(m)$ when we want to emphasize it is as an on-site energy.] The interpretation of these equations is exactly the same as in the continuum case. Thus, $\mathcal{H}_{sc}(q, m)$ is a semiclassical Hamiltonian, $q(m)$ is a local wavevector as already mentioned, and $v(m)$ is the associated semiclassical electron velocity. We shall refer to Eq. (1.5) as the basic DPI form. Equation (1.6) is the eikonal or Hamilton-Jacobi equation, while Eq. (1.7) is the discrete counterpart of the transport equation. The presence of the lattice shows up in the $q$ dependence of $\mathcal{H}_{sc}(q, m)$ through periodic functions, whereas in the continuum case, such dependence is typically of the form $q^2$.

As discussed by Braun [34], the DPI approximation has been employed in many problems in quantum mechanics where the Schrödinger equation turns into a three-term recursion relation in a suitable basis. All the types of problems as in the continuum case in can then be treated—Bohr-Sommerfeld quantization, barrier penetration, tunnel in symmetric double
wells, etc. In addition, one can also use the method to give asymptotic solutions for various recursion relations of mathematical physics, such as those for the Mathieu equation, Hermite polynomials, Bessel functions, and so on. The general procedures are well known and simple to state. For any \(E\), one solves the Hamilton-Jacobi and transport equations to obtain \(q(m)\) and \(v(m)\), and writes \(C_m\) as a linear combinations of the independent solutions that result. The interesting features all arise from a single fact — that the DPI approximation breaks down at the so-called turning points. These are points where \(v(m)\) vanishes. One must relate the DPI solutions on opposite sides of the turning point by connection formulas, and the solution of all the various types of problems mentioned above depends on judicious use of these formulas.

In this paper we will extend these ideas to five-term recursion relations, focussing especially on those features which arise over and above the three-term problem. Now, for any given \(E\), there will be four DPI solutions \([1,5]\), while in the three-term case there are only two, because the Hamilton-Jacobi equation \([1,6]\) is a quartic in \(e^{iq}\). These solutions will also break down at turning points—points where \(v(m)\) vanishes. In contrast to the three-term case, we shall see that there are new types of turning points. It is these turning points which are responsible for the diabolical points in the spectrum of \(Fe_8\). The three-term problem turning points are analogous to those in the continuum quasiclassical method, but the new ones that we will find are not. In fact, they can only be described as lying “under the barrier” from the continuum viewpoint. These new or irregular turning points require new connection formulas, which it is our goal to provide.

The plan of our paper is as follows. We will examine the DPI approximation carefully in Sec. II, and see how it fails when \(v(m)\) vanishes. The precise width of the failure zone is discussed in an Appendix. We will examine these failure or turning points in Sec. III and see how the concept must be extended beyond the three-term and continuum cases. We will find that a turning point need not be a limit of the classically allowed motion, and we will categorize the different types of turning points that arise. We will conclude in Sec. IV by deriving connection formulas at the new turning points.

We will limit ourselves to problems where the matrix \(t_{m,n}\) is real and symmetric, \(t_{m,n} = t_{n,m}\), as it simplifies the analysis, and yet suffices to bring out all essential physical points. In our spin example, this means that we only consider fields in the \(x-z\) plane. The extension to complex Hermitean matrices is cumbersome to carry through, but presents no difficulty of principle. We shall continue to couch our discussion in quantum mechanical language, thinking of \(E\) as an energy eigenvalue, although from the mathematical viewpoint, this is not strictly necessary.

II. THE BASIC DPI APPROXIMATION

In this section, we will examine the DPI approximation in more detail. The argument proceeds in close analogy with the continuum case. We begin by restating the approximation in a slightly different way \([4,12]\). Dividing Eq. (1.2) by \(C_m\), and writing \(\zeta_{m+1} = C_{m+1}/C_m\), we get

\[
t_{m,m-2}\zeta_{m-1}^{-1}\zeta_m^{-1} + t_{m,m-1}\zeta_m^{-1} + t_{m,m} + t_{m,m+1}\zeta_{m+1} + t_{m,m+2}\zeta_{m+1}\zeta_{m+2} = E. \tag{2.1}
\]
If $t_{m,m+\alpha}$ for fixed $\alpha$ is almost the same over some range $K \gg 1$ of $m$’s, then we will get almost the same numerical equation for the $\zeta_m$’s over this range, and we will clearly obtain a good approximate solution if we replace ratios like $\zeta_{m+1}/\zeta_m$ by unity. This leads to

$$t_{m,m-2}\zeta_m^2 + t_{m,m-1}\zeta_m^{-1} + t_{m,m} + t_{m,m+1}\zeta_m + t_{m,m+2}\zeta_m^2 = E,$$

(2.2)

which is a solvable quartic equation in $\zeta_m$ (which is exactly like the factor $e^{iq(m)}$ introduced in Sec. [I]). The corresponding approximation for $C_m$ is

$$C_m \approx \prod_{k=m_a}^{m} \zeta_k,$$

(2.3)

where $m_a$ is a suitable starting value. One could now use this approximation to find the ratio $\zeta_{m+1}/\zeta_m$, substitute this value for the ratio in Eq. (2.1), and solve again for $\zeta_m$. The process could be further iterated if desired.

The product in Eq. (2.3) is more easily evaluated as a sum by taking logarithms. Further, if the $\zeta_m$’s do not vary rapidly from one $m$ to the next, the sum will be well approximated by an integral. This makes it necessary to introduce continuum extensions of the matrix elements $t_{m,m+\alpha}$. We turn therefore to this problem, and discuss the condition for slow variation more clearly. We are seeking functions $t_\alpha(m)$ such that

$$t_\alpha(m) = (t_{m,m+\alpha} + t_{m,m-\alpha})/2, \quad (\alpha = 0, 1, 2),$$

(2.4)

whenever $m$ is an integer. There are infinitely many such functions, and we restrict them by imposing further conditions on a certain number of their higher derivatives. For $t_1(m)$, e.g., we could also demand (using dots to denote derivatives with respect to $m$),

$$\dot{t}_1(m) = t_{m,m+1} - t_{m,m-1},$$

$$\ddot{t}_1(m) = \frac{1}{2} (t_{m+1,m+2} - t_{m,m+1} - t_{m,m-1} + t_{m+1,m+2}).$$

(2.5)

(2.6)

Similar conditions can be imposed on $t_0(m)$ and $t_1(m)$. In general, we need conditions only up to some small order for practical applications. Up to the degree of approximation in Eq. (1.3), e.g., we need only go up to second derivatives.

Since the matrix elements are assumed to vary slowly, we want these derivatives to be small, and this condition is best codified in terms of a small parameter $\epsilon$, which plays the same role as $\hbar$ in the continuum case, such that $t_\alpha$ is formally of order $\epsilon^0$, $\dot{t}_\alpha$ of order $\epsilon$, $\ddot{t}_\alpha$ of order $\epsilon^2$, and so on. For spin Hamiltonians such as Eq. (1.1), this parameter is $1/J$. The quasiclassicality conditions then read

$$\frac{dt_\alpha}{dm} = O\left(\frac{t_\alpha(m)}{J}\right), \quad \frac{d^2t_\alpha}{dm^2} = O\left(\frac{t_\alpha(m)}{J^2}\right),$$

(2.7)

etc. We will continue to use $1/J$ as a generic small parameter in the rest of our analysis. A problem in which one can not find functions $t_\alpha(m)$ obeying Eq. (2.7) will not be amenable to a phase integral approximation.

One small point should be kept in mind while judging orders of smallness in the spin problem, and others like it. There are natural algebraic expressions for the $t_\alpha(m)$’s in which
m appears only in the combination \( m/J \) or \( m/[J(J+1)]^{1/2} \). Thus, derivatives with respect to \( m \) are automatically smaller by an order \( J^{-1} \). As \( J \to \infty \), however, the classical quantity is not \( m \), but \( m/J \). Thus the ratio \( m/J \) should be regarded as a quantity of order unity and not \( J^{-1} \).

With this lengthy preamble, we are ready to solve our recursion relation. As in the continuum case, we make the exponential substitution,

\[
C_m = e^{i\Phi(m)}. \tag{2.8}
\]

The first approximation is obtained if we assume that \( \dot{\Phi}(m) \) varies slowly so that \( \ddot{\Phi}(m) \) may be neglected. Then \( C_{m\pm\alpha} \approx C_m e^{i\alpha\Phi} \), and substituting this into the recurrence relation with \( t_{m,m\pm\alpha} \approx t_\alpha(m) \), we obtain the Hamilton-Jacobi equation with \( \dot{\Phi}(m) = q(m) \).

To proceed more systematically, we look for a solution for \( \Phi(m) \) as a series in inverse powers of \( J \):

\[
\Phi = \Phi_0 + \Phi_1 + \Phi_2 + \cdots, \tag{2.9}
\]

where,

\[
\begin{align*}
\Phi_n &= O(J^{1-n}), \\
\dot{\Phi}_n &= O(\Phi_n/J), \\
\ddot{\Phi}_n &= O(\Phi_n/J^2),
\end{align*}
\tag{2.10}
\]

and so on. The successive inverse powers of \( J \) in the derivatives are expected since we expect the \( \Phi_n \) to be simple functions of the \( t_{m,m+\alpha} \), and we shall soon see whether or not this expectation is fulfilled. \( \Phi_0 \) is our zeroth order approximation above, and so we set

\[
\dot{\Phi}_0(m) = q(m) \tag{2.11}
\]

from the outset. As in the continuum case, we need to keep terms up to \( \Phi_2 \) in order to decide if the approximation is succeeding.

Up to terms of order \( 1/J^2 \) relative to the leading one, we have

\[
C_{m\pm1} = C_m \exp \left[ i \left( \pm q \pm \dot{\Phi}_1 \pm \dot{\Phi}_2 + \frac{1}{2}(\ddot{q} + \ddot{\Phi}_1) \pm \frac{1}{6} \dddot{q} + \cdots \right) \right]
= C_m e^{\pm i q} \left[ 1 + \frac{i}{2}(\ddot{q} \pm 2\dot{\Phi}_1) - \frac{1}{8}(\ddot{q} \pm 2\dot{\Phi}_1)^2 \pm i\dot{\Phi}_2 + \frac{i}{2} \dddot{\Phi}_1 \pm \frac{i}{6} \dddot{q} + \cdots \right]. \tag{2.12}
\]

We now wish to substitute this form into our recursion relation. We would like to use the continuum forms \( t_\alpha(m) \) instead of the discrete matrix elements \( t_{m,m+\alpha} \). Just as there are infinitely many continuous functions which we could take, there are many approximants for \( t_{m,m+\alpha} \). Note in particular, that there is no unique way to “solve” Eqs. (2.4) – (2.6) for the matrix elements in terms of the continuous functions. The simplest procedure is to take \( t_{m,m} = t_0(m) \), \( t_{m,m\pm1} = t_1(m \pm \frac{1}{2}) \), and \( t_{m,m\pm2} = t_2(m \pm 1) \). For \( t_{m,m\pm1} \), in particular, a Taylor expansion of this approximation gives

\[
t_{m,m\pm1} = t_1(m) \pm \frac{i}{2} t_1(m) + \frac{1}{8} i t_1(m) + \cdots, \tag{2.13}
\]
where the error is of order $J^{-3}$. Therefore,

$$\sum_{n=m \pm 1} t_{m,n} C_n = t_1(m)\alpha_1(m) + \dot{t}_1(m)\alpha_2(m) + \ddot{t}_1(m)\alpha_3(m) + \cdots, \quad (2.14)$$

where

$$\alpha_1(m) = 2C_m \left[ \cos q + \frac{i}{2} (\dot{q} \cos q + 2i\dot{\Phi}_1 \sin q) - \frac{1}{8} \left( \dot{q}^2 + 4\dot{\Phi}_1^2 - 4i\ddot{\Phi}_1 \right) \cos q \right. \left. - \frac{i}{6} \left( 3\dot{q}\dot{\Phi}_1 - 6i\dddot{\Phi}_2 - i\dddot{q} \right) \sin q \right],$$

$$\alpha_2(m) = iC_m \left[ \sin q + \frac{i}{2} \dot{q} \sin q + \dot{\Phi}_1 \cos q \right], \quad (2.15)$$

$$\alpha_3(m) = \frac{1}{4} C_m \cos q.$$ 

Note that we have kept only terms up to order $1/J^2$ in $\alpha_1$, $1/J$ in $\alpha_2$, and $J^0$ in $\alpha_3$, since relative to $t_1(m)$, $\dot{t}_1$ and $\ddot{t}_1$ are of order $1/J$ and $1/J^2$, respectively.

Similarly,

$$\sum_{n=m \pm 2} t_{m,n} C_n = t_2(m)\beta_1(m) + \dot{t}_2(m)\beta_2(m) + \ddot{t}_2(m)\beta_3(m) + \cdots, \quad (2.16)$$

where

$$\beta_1(m) = 2C_m \left[ \cos 2q + 2i \left( \dot{q} \cos 2q + i\dot{\Phi}_1 \sin 2q \right) - 2 \left( \dot{q}^2 + \dot{\Phi}_1^2 - i\ddot{\Phi}_1 \right) \cos 2q \right. \left. - \frac{2i}{3} \left( 6\dot{q}\dot{\Phi}_1 - 3i\dddot{\Phi}_2 - 2i\dddot{q} \right) \sin 2q \right],$$

$$\beta_2(m) = 2iC_m \left[ \sin 2q + 2i\dot{q} \sin 2q + 2\dot{\Phi}_1 \cos 2q \right], \quad (2.17)$$

$$\beta_3(m) = C_m \cos 2q.$$ 

We now substitute these relations into the recurrence relation (1.2), and equate equal powers of $J$. The terms of order $J^0$ obviously give Eq. (1.6), while those of order $J^{-1}$ give, after some work,

$$-2\dot{\Phi}_1 (t_1 \sin q + 2t_2 \sin 2q) = -i \frac{d}{dm} (t_1 \sin q + 2t_2 \sin 2q). \quad (2.18)$$

The left hand side of this equation is $\dot{\Phi}_1 v(m)$ [see Eq. (1.7)], while the right hand side may be written as $(i/2)dv(m)/dm$. Thus, integration yields (after a suitable choice of an indefinite constant)

$$\Phi_1(m) = \frac{i}{2} \ln v(m). \quad (2.19)$$

Note that as assumed in Eq. (2.10), $\Phi_1 = O(J^0)$. Pending a demonstration that $\Phi_2(m)$ is negligible, we have arrived at the basic DPI form (1.5), which we now see as the first two terms of an asymptotic expansion of $\Phi$ in inverse powers of $J$.

The equation for $\Phi_2(m)$ is considerably more involved. After some analysis, we find
\[ \frac{d\tilde{\Phi}_2}{dm} = \frac{1}{8} \frac{d^2 r}{dm^2} + i \frac{d\Phi_1}{4 dm}, \]  
where we have defined
\[ \tilde{\Phi}_2 = \Phi_2 + \frac{1}{24} \int \frac{t_1 + 16 t_2 \cos q}{t_1 + 4 t_2 \cos q} \dot{q} dm, \]  
(2.21)
\[ r(m, q(m)) = \frac{t_1 \cos q + 4 t_2 \cos 2q}{t_1 \sin q + 2 t_2 \sin 2q}. \]  
(2.22)
Thus,
\[ \Phi_2 = -\frac{1}{24} \int \frac{t_1 + 16 t_2 \cos q}{t_1 + 4 t_2 \cos q} \dot{q} dm + \frac{1}{8} \frac{dr}{dm} - \frac{1}{8} \int r \frac{d^2 \ln v}{dm^2} dm. \]  
(2.23)
Based on power counting, this is indeed of order \( J^{-1} \), since \( \dot{q} \) and \( d^2 \ln v(m)/dm^2 \) are of order \( J^{-2} \). Thus, \( |\Phi_2| \ll \Phi_1 = O(J^0) \). However, it is plain that this condition is violated whenever \( v(m) \) approaches zero, for then both \( \ln v(m) \) and \( r(m) \) diverge. To find the actual magnitude of \( \Phi_2 \), we need to know how \( q(m) \) and \( v(m) \) behave near a turning point. This behavior is found in the next section [see Eqs. (3.14) and (3.15)]. The magnitude of \( \Phi_2 \) is estimated in Appendix A, where we show that the width of the zone where DPI fails is of order \( J^{1/3} \).

III. TURNING POINTS

We now turn to a study of the points where \( v(m) = \partial H_{sc}(q, m) / \partial q = 0 \). We shall call all such points turning points in analogy with the continuum case. In contrast to that case, however, we will find that turning points are not just the limits of the classical motion for a given energy, once the notion of the classically accessible region is suitably understood.

Since we must also obey the eikonal equation (1.6) in addition to the condition \( v(m) = 0 \), at a turning point both \( m \) and \( q \) are determined if \( E \) is given. Setting \( v = 0 \) in Eq. (1.7), we see that we must have either \( q = 0 \), or \( q = \pi \), or \( q = q_\star(m) \), where
\[ \cos q_\star(m) = -\frac{t_1(m)}{4 t_2(m)}. \]  
(3.1)
Substituting these value of \( q \) in the eikonal equation, we see that a turning point arises whenever
\[ E = U_0(m), \ U_\pi(m), \text{ or } U_\star(m), \]  
(3.2)
where,
\[ U_0(m) = H_{sc}(0, m) = w(m) + 2 t_1(m) + 2 t_2(m), \]  
(3.3)
\[ U_\pi(m) = H_{sc}(\pi, m) = w(m) - 2 t_1(m) + 2 t_2(m), \]  
(3.4)
\[ U_\star(m) = H_{sc}(q_\star, m) = w(m) - 2 t_2(m) - \frac{t_1^2(m)}{4 t_2(m)}. \]  
(3.5)
Note that \( q_\star(m) \) may be complex for some \( m \), but since \( \cos q_\star \) is always real, \( U_\star \) is real for all \( m \). We shall refer to these three energy curves as critical curves.
In the one-dimensional continuum case where $\mathcal{H}_{sc} = (p^2/2m) + V(x)$, the condition $v(x) = 0$ is equivalent to $E = V(x)$. The latter condition marks the edge of the classically allowed region, $E < V(x)$. Let us recall why this is said to be so. A particle at a point $x$ where $V(x) > E$ must be ascribed an imaginary momentum. To understand the analogous condition in the discrete case, let us return to the analogy of an electron in a one-dimensional lattice with $m$-independent matrix elements $t_{m,m+a}$. Equation (1.3) gives the dispersion relation for an energy band $E(q)$. The classically allowed range of energies is now defined by the limits of this band since (provided one is not too close to a band edge) a spatially localized electron with a mean energy in this range can be constructed as a wavepacket out of Bloch states with only real wavevectors. Alternatively, we could say that solutions with energy in the allowed range correspond to travelling waves, while solutions outside this range correspond to evanescent waves. These notions continue to be valid when $t_0(m)$ are slowly varying with $m$. The dispersion relation may be taken as $\mathcal{H}_{sc}(q,m)$ for any fixed value of $m$. The band is now $m$-dependent, and so in particular are the band edges, which we denote by $U_-(m)$ (lower edge) and $U_+(m)$ (upper edge).

To find the band edges, we note that by definition, the energy at an edge is either a minimum or maximum, so $\partial \mathcal{H}_{sc}(q,m)/\partial q = 0$, i.e., $v(m) = 0$. [The converse is not true, i.e., $v(m) = 0$ need not always define a band edge.] Thus the wavevectors at the band edges are again to be found in the set $q = 0$, $\pi$, and $q_s$, with the answers depending on the signs and magnitudes of $t_1$ and $t_2$. [We do not distinguish between $q = \pi$ and $q = -\pi$, or between $q = q_s$ and $q = -q_s$, as $\mathcal{H}_{sc}(q,m)$ is an even function of $q$.] To narrow down the number of cases to be considered, we observe that the gauge transformation $C_m \rightarrow (-1)^m C_m$ changes the sign of $t_1$. Hence, we may assume $t_1 < 0$ without loss of generality. Consider the case $t_2 > 0$ first. Then the upper band edge is always located at $q = \pi$, while the lower band edge is located at $q = 0$ if $t_1/4t_2 < -1$, and at $q_s = \cos^{-1}(-t_1/4t_2)$ if $-1 < t_1/4t_2 < 0$. The case $t_2 < 0$ is completely analogous. Now the lower band edge is always at $q = 0$, while the upper band edge is at $q = \pi$ for $t_1/4t_2 > 1$, and at $q_s = \cos^{-1}(-t_1/4t_2)$ for $0 < t_1/4t_2 < 1$. The different types of band energy curves that can arise are illustrated in Fig. 1. In the rest of this paper we shall carry out the analysis in detail assuming $t_2 > 0$. The case $t_2 < 0$ is easily treated in parallel, and we shall only give the final results where these are significantly different.

The conditions Eq. (1.2) for a turning point are analogous to the requirement that $E = V(x)$ in the continuum case. Correspondingly, it helps in visualization to draw all three critical curves versus $m$, and a horizontal line indicating the energy. Any intersection of this line with a critical curve is a turning point. See, e.g., Figs. 2 and 3.

Not every critical curve need be a band edge curve, however. Since we have chosen $t_1(m) < 0$ and $t_2(m) > 0$, the upper edge curve $U_+(m)$ is the same as $U_+(m)$ for all $m$, but the lower edge curve, $U_-(m)$, may be $U_0(m)$ for some values of $m$, and $U_+(m)$ for other values as discussed above. It turns out to be useful to introduce a dual labelling scheme for the critical curves and write

\begin{equation}
U_0(m) = U_1(m), \quad U_+(m) = U_-(m), \quad \text{if } q_s \in (0, \pi),
\end{equation}
\begin{equation}
U_0(m) = U_-(m), \quad U_+(m) = U_f(m), \quad \text{if } q_s \notin (0, \pi).
\end{equation}

We have already noted that $U_+(m) = U_+(m)$. The subscripts $i$ and $f$ stand for “internal” and “forbidden”, since in the first case above, $U_0(m)$ lies inside the classically allowed energy
range, while in the second case, \(U_*(m)\) lies outside this range. The turning points with \(E = U_i\) and \(E = U_f\) have no analogues in continuum quantum mechanical problems.

Before turning to a classification of the various turning points, however, it is useful to record some further properties of the critical curves. The first property is that \(U_0(m) \geq U_*(m)\), since

\[
U_0(m) - U_*(m) = \frac{1}{4t_2(m)}(t_1(m) + 4t_2(m))^2.
\]

Differentiating this equation with respect to \(m\), it follows that the case of equality, \(U_0(m) = U_*(m)\), happens at a point where both curves have a common tangent. These facts are illustrated in Fig. 4. Further, at the point of contact, which we denote by \(m^*, t_1(m)/4t_2(m) = -1\), which is precisely the condition derived above for the lower band edge to change from \(q = 0\) to \(q = q_*\).

The second property provides an alternative way of viewing the condition \(E = U_*(m)\). Solving the eikonal equation (1.6) for \(\cos q\) we obtain

\[
\cos q(m) = \frac{-t_1(m) \pm [t_1^2(m) - 4t_2(m)f(m)]^{1/2}}{4t_2(m)};
\]

\[
f(m) = w(m) - 2t_2(m) - E.
\]

Since \(\cos q = -t_1/4t_2\) at \(q = q_*\), the discriminant in Eq. (3.9) must vanish, and we must have

\[
t_1^2(m) = 4t_2(m)(w(m) - 2t_2(m) - E) \quad (q = q_*).
\]

It is easily verified that this equality is identical to \(E = U_*(m)\).

We now turn to discussing the different types of turning points:

**Type A:** \(E = U_-(m)\) when \(U_- = U_0\). See, e.g., Fig. 2. The region \(m \leq m_c\) is classically allowed. This is analogous to what happens in the conventional continuum quasiclassical method — the turning point is located at the boundary of the classically accessible region for the energy given. For \(m\) just less than \(m_c\), there are two solutions of the Hamilton-Jacobi equation (1.4) with \(q \approx [(E - U_-(m))/a]^{1/2}\), where \(a = -(t_1 + 4t_2)\). For \(m\) just greater than \(m_c\), these values of \(q\) continue on to the imaginary axis. The corresponding wavefunctions \(C_m\) change from slowly oscillatory for \(m < m_c\) to exponentially growing and decaying for \(m > m_c\). The connection formulas for these solutions are exactly like those in the continuum case, and may be derived as in Refs. 2,3. Note that the other two solutions of the Hamilton-Jacobi equation evolve smoothly, and the corresponding DPI wavefunctions \(C_m\) do not need to be “connected” across this turning point.

**Type A:** \(E = U_+(m)\). See Fig. 2 again. The region \(m \geq m_b\) is classically allowed. This case is physically very similar to type A in that the turning point is at the boundary of the classically allowed and forbidden regions. Now, however, \(q \approx \pi\) in the transition zone, so the wavefunctions contain a rapidly oscillating factor \((-1)^m\) in addition to all the other variation. Although the connection formulas can be derived from those for type A turning points by means of the transformation \(C_m \rightarrow (-1)^m C_m\), as shown in Ref. 3, their detailed form has a very different superficial look.
Type A': $E = U_1(m)$. Consider Fig. 3, and the energy $E$ shown there, which intersects $U_1(m)$ at $m = m_c$. In Fig. 3 we sketch energy bands for this problem for several values of $m$. For $m$ just less than $m_c$, $H_{sc}(q, m) = E$ in just two places, which we denote by $\pm q(m)$. (We do not show the solution $-q(m)$ explicitly.) For $m$ just greater than $m_c$, two new intersections develop at $\pm q^*(m) \approx 0$. Thus for $m > m_c$, our wavefunction consists of a sum of four basic solutions $[\text{Eq. (1.5)}]$, all oscillatory, while for $m < m_c$ we have two oscillatory solutions [associated with $\pm q(m)$], and two exponentially decaying or growing solutions [associated with $\pm q^*(m)$].

The latter solutions must be related across the turning point by connection formulas, which are completely identical to those for type A. The fact that we may have exponentially decaying and growing solutions inside a classically allowed region is unexpected from prior experience with the continuum quantum mechanical problems, and underscores the point that this turning point has no analogue there. We are unaware if it has ever been considered in other physical situations where a continuum phase integral approach may be applied.

Type B: $E = U_f(m)$. This turning point is perhaps the most interesting of all. Since the energy now lies outside the classically allowed range, the point lies “under the barrier”, and at it, $q$ must be purely imaginary. Consider Fig. 4, and the energy $E$, which intersects $U_f$ at $m = m_c$. We see that for $m \leq m_c$, there are two solutions to the Hamilton-Jacobi equation $[\text{Eq. (1.5)}]$ with $q = \pm i \kappa$, where $\kappa$ is real. For $m > m_c$, these solutions acquire a real part as well, so that $C_m [\text{See Eq. (1.5)}]$ changes from a decaying (or growing) exponential to an oscillating solution with an exponentially decaying (or growing) envelope. As for type A’ points, this behavior has no analogue in continuum quantum mechanical problems, and we are unaware of prior analyses in other contexts. We shall derive connection formulas for this case in Sec. IV.

Type B': $E = U_-(m)$ when $U_-(m) = U_*(m)$. This turning point is like type A in that the energy lies at the lower limit of the classically allowed region, but like type B in that $q \neq 0$. The solutions which must be connected are purely oscillatory on the classically allowed side, with $q \approx \pm q_*$, and oscillatory exponentials (growing or decaying) on the forbidden side. The connection formulas are similar to those for case B.

Our nomenclature for the turning points may have become evident to the reader. The letter A indicates that $q = 0$ or $\pi$, while B indicates that $q = q^*$. A bar designates cases where $q$ has a value close to $\pi$, leading to a oscillatory factor in $C_m$ close to $(-1)^m$, and a prime indicates cases where $U_*$ is either $U_-$ or $U_+$ at the turning point value of $m$. Thus in the case $t_1 < 0, t_2 < 0$, we would have turning points of type A, $\tilde{A}$, $\tilde{B}$, and $\tilde{B}'$. Note that the mathematical aspects of the turning point, i.e., connection formulas, are governed by the value of $q$ at the turning point, but its physical nature is governed by whether the energy lies at the boundary (cases A, $\tilde{A}$, $\tilde{B}$, and $\tilde{B}'$), in the interior (cases A’ and $\tilde{A}'$), or in the exterior (cases B and $\tilde{B}$) of the classically allowed range.

It will now be apparent that in problems with three-term recursion relations, where $H_{sc}(q, m) = w(m) + 2t_1(m) \cos q$, and $v(m) = -2t_1(m) \sin q(m)$, the only turning points are at band edges, with $q = 0$ or $\pi$, i.e., of type A or A’. It is also apparent that no new points are involved in problems with further neighbor hopping, i.e., recursion relations with seven or more terms. Turning points are encountered whenever the energy lies on a critical curve, where this term now describes all curves in the $E$-$m$ plane on which $\partial H_{sc}(q, m)/\partial q = 0$. As $m$ is varied through each turning point, two roots of the Hamilton-Jacobi equation for $q$ approach each other parallel to either the real or imaginary axis, coalesce, and move apart
in the orthogonal direction [17]. Consider for example the band structure in Fig. 6, which could arise from a recursion relation with seven or more terms. The accompanying critical curves are shown in Fig. 7. For the energy $E$ shown, if $m < m_a$, there is only one real solution for $q$, i.e. $q_+$. (We do not explicitly mention negative values of $q$.) At $m = m_a$, a new real value of $q$, $q_2$, enters the picture, and splits into two solutions $q_{2-}$ and $q_{2+}$ as $m$ increases further.

We conclude this section by finding the general behavior of $q(m)$ and $v(m)$ near a turning point $m = m_c$. In its vicinity we may write

$$H_{sc}(q, m) = H_{sc}(q, m_c) + (m - m_c) \frac{\partial H_{sc}}{\partial m}\bigg|_{m_c} + \cdots.$$  \hspace{1cm} (3.12)

By definition, however, $v(m_c) = 0$, and so $H_{sc}(q, m) - E$, and $\partial[H_{sc}(q, m_c) - E]/\partial q$ both vanish. If we write $q(m_c) = q_c$, expand the right hand side of Eq. (3.12) in powers of $q - q_c$ as well, and retain only the leading non vanishing terms in $q - q_c$ and $m - m_c$, we obtain

$$H_{sc}(q, m) - E \approx a(q - q_c)^2 + b(m - m_c) + \cdots,$$  \hspace{1cm} (3.13)

where $a$ and $b$ are constants. If we regard $w(m)$ and $t_\alpha(m)$ as being of order $J^0$, then by Eq. (2.7), we have $a = O(J^0)$, and $b = O(1/J)$, and therefore

$$q(m) - q_c \sim [(m - m_c)/J]^{1/2},$$  \hspace{1cm} (3.14)

$$v(m) \sim [(m - m_c)/J]^{1/2}.$$  \hspace{1cm} (3.15)

These formulas prove useful when connection formulas are derived. Their usefulness is limited, however, if there is another turning point very close to $m_c$. In this case we should keep terms of order $(m - m_c)^2$. The requisite analysis is very similar to that of quadratic turning points [18] in the continuum case, but we shall not have any occasion to pursue it further. In all the calculations we have done for the Fe$_8$ or other spin problems [19], we have been able to sidestep the associated quadratic connection formulas by directly matching the solutions in the forbidden region to solutions of the Schrödinger equation for a harmonic oscillator.

**IV. CONNECTION FORMULAS FOR FORBIDDEN REGION TURNING POINTS**

We turn at last to the problem of finding connection formulas at the turning points. The formulas for points of type $A$, $\bar{A}$, etc. are quoted by Braun [3], so we will only consider points of type $B$ and $\bar{B}$. Our procedure is a small modification of that used by Schulten and Gordon [2]. Suppose the turning point is at $m = m_c$, and $q(m_c) = q_c$. As shown in Appendix A, the DPI solution (1.5) fails in a window $\Delta m \equiv |m - m_c| \leq O(J^{1/3})$, which we shall refer to as the failure zone. The first step is therefore to find another approximation that holds in the larger window (which we refer to as the central zone) $\Delta m \ll J^\eta$, where $\eta > 1/3$. To do this we write $C_m$ as an $e^{i\eta \cdot m}$ times a slowly varying factor, $y_m$, for which we then derive an approximate second order differential equation. The second step is to asymptotically match solutions
of this differential equation to the DPI solutions in the overlap zones $J^n \gg \Delta m \gg J^{1/3}$ on either side of the turning point where both types of solutions are valid. The last step is to directly write down the transformation matrix between the coefficients of the linear combination of DPI solutions for $m < m_c$ to those for $m > m_c$, without having to consider the solution in the intermediate zone. We will carry out these three steps only to an order necessary to match the solutions to the accuracy represented by Eq. (1.5), i.e., to order $J^0$ in the phase $\Phi(m)$ introduced after Eq. (1.2) or in Eq. (2.8).

Let us assume as before that $t_1 < 0$, $t_2 > 0$, and first consider turning points of type $B$. We will denote quantities evaluated at $m = m_c$ by a subscript $c$: $t_1(m_c) = t_{1c}$, $\dot{t}_1(m_c) = \dot{t}_{1c}$, etc. Let $q$ be pure imaginary for $m \leq m_c$, and precisely at $m_c$ let us write

$$q(m_c) = i\sigma_2\kappa_c,$$

(4.1)

where $\kappa_c > 0$ and $\sigma_2 = \pm 1$. Putting this in Eqs. (3.1) and (1.6) we have

$$t_{1c} = -4t_{2c} \cosh \kappa_c,$$

(4.2)

$$E = w_c + 2t_{1c} \cosh \kappa_c + 2t_{2c} \cosh 2\kappa_c,$$

(4.3)

To carry out step 1, we write

$$C_m \approx e^{-\sigma_2\kappa_c(m-m_c)}\dot{y}(m),$$

(4.4)

where $\dot{y}(m) \ll \kappa_c$. Assuming that this is so, we write

$$C_{m \pm k} = e^{-\sigma_2\kappa_c(m-m_c)}e^{-\sigma_2\kappa_c k}[y \pm k\dot{y} + \frac{1}{2}k^2\ddot{y} + \cdots].$$

(4.5)

This approximation will hold provided $\dot{y} \ll y$, and $\ddot{y} \ll \dot{y}$ throughout the central zone $|m - m_c| \ll J^n$. [We anticipate, in fact, that throughout this zone, $\dot{y}(m) \sim J^{-\gamma}y(m)$ where $\gamma > 0$.] That this is so and that higher order derivatives can be neglected in Eq. (4.5) will be justified post facto. Substituting Eq. (4.3) in Eq. (1.2) we obtain

$$A_0(m)\ddot{y}(m) + A_1(m)\dot{y}(m) + A_2(m)y(m) \approx 0,$$

(4.6)

where

$$A_0 = \sum_{k=\pm1,\pm2} \frac{1}{2}k^2e^{-\sigma_2\kappa_c t_{m,m+k}},$$

(4.7)

$$A_1 = \sum_{k=\pm1,\pm2} ke^{-\sigma_2\kappa_c t_{m,m+k}},$$

(4.8)

$$A_2 = \sum_{k=\pm1,\pm2} e^{-\sigma_2\kappa_c t_{m,m+k}} + w_m - E,$$

(4.9)

The differential equation that we are seeking for $y(m)$ need only hold in window of width $O(J^n)$ with $\eta > 1/3$ around $m_c$. If we choose $\eta < 1$, we can use the fact that $w(m)$ and $t_\alpha(m)$ are slowly varying, and use the expansions

$$t_{m,m \pm k} \approx t_k(m) \pm \frac{1}{2}k\dot{t}_k(m),$$

(4.10)

$$t_k(m) \approx t_{kc} + (m - m_c)t_{kc},$$

(4.11)
etc. Doing this, we obtain

\[ A_0 \approx a_1, \quad (4.12) \]
\[ A_1 \approx a_2 - \sigma_2 (m - m_c) b_2, \quad (4.13) \]
\[ A_2 \approx -\sigma_2 a_3 + (m - m_c) b_3, \quad (4.14) \]

where

\[ a_1 = t_{1c} \cosh \kappa_c + 4t_{2c} \cosh 2\kappa_c, \quad (4.15) \]
\[ a_2 = \dot{t}_{1c} \cosh \kappa_c + 4\dot{t}_{2c} \cosh 2\kappa_c, \quad (4.16) \]
\[ b_2 = 2 \sinh \kappa_c (\dot{t}_{1c} + 4\dot{t}_{2c} \cosh \kappa_c), \quad (4.17) \]
\[ a_3 = \sinh \kappa_c (\dot{t}_{1c} + 4\dot{t}_{2c} \cosh \kappa_c) = \frac{1}{2} b_2, \quad (4.18) \]
\[ b_3 = \dot{w}_c + 2\dot{t}_{1c} \cosh \kappa_c + 2\dot{t}_{2c} \cosh 2\kappa_c, \quad (4.19) \]

and where we used Eq. (1.3) to simplify the expression for \( A_2 \). We can also simplify the results for \( a_1 \) and \( b_3 \). Using Eq. (4.2) in Eq. (4.15), we obtain

\[ a_1 = 4t_{2c} \sinh^2 \kappa_c > 0. \quad (4.20) \]

To simplify \( b_3 \), we recall that the discriminant in Eq. (3.9) vanishes at \( m = m_c \). Expanding about \( m_c \), we have

\[ t_2^2(m) - 4t_2(m) f(m) = -\frac{16}{J} \alpha^2(m - m_c) t_{2c}^2 + O((m - m_c)/J)^2, \quad (4.21) \]

where \( \alpha \) is a positive constant. Differentiating with respect to \( m \) and setting \( m = m_c \), we obtain

\[ t_{1c} \dot{t}_{1c} - 2t_{2c} \dot{f}_c - 2t_{2c} f_c = -\frac{8}{J} \alpha^2 t_{2c}^2. \quad (4.22) \]

Since \( f = w - 2t_2 - E \), using Eqs. (1.3) and (4.2), we obtain \( f_c = 4t_{2c} \cosh^2 \kappa_c \). Also, \( \dot{f}_c = \dot{w}_c - 2\dot{t}_{2c} \), and the left hand side of Eq. (4.22) becomes

\[ -2t_{2c} (\dot{w}_c + 2\dot{t}_{1c} \cosh \kappa_c + 2\dot{t}_{2c} \cosh 2\kappa_c), \quad (4.23) \]

which by Eq. (1.19) we recognize as \(-2t_{2c} b_3 \). Therefore,

\[ b_3 = 4\alpha^2 t_{2c}/J. \quad (4.24) \]

One can also similarly show that

\[ a_3 = t_{2c} \sinh \kappa_c \frac{d}{dm} \left( \frac{t_{1c}}{t_{2c}} \right) \bigg|_{m=m_c}, \quad (4.25) \]

but this result is not particularly useful.

Let us now examine the order of magnitude of the various \( a \) and \( b \) coefficients just introduced. We first note that since \( t_{ac} = O(J^0) \) and \( t_{ac} = O(J^{-1}) \), Eq. (1.22) implies that \( \alpha = O(1) \). It follows that \( a_1 = O(J^0) \), while \( a_2, a_3, b_2, \) and \( b_3 \) are all of order \( J^{-1} \).
To solve the differential equation (4.6) with the approximations (4.12)–(4.14) for the A’s, we eliminate the first derivative via the substitution

\[ y(m) = z(m) \exp -\frac{1}{2a_1} \left[ a_2(m - m_c) - \frac{b_2}{2} \sigma_2(m - m_c)^2 \right]. \] (4.26)

Then \( z(m) \) obeys

\[ a_1 \ddot{z}(m) + b'_3(m - m'_c)z_m = 0, \] (4.27)

where we have dropped a term of order \((m - m_c)^2/J^2\) in the coefficient of \(z_m\), and where

\[ b'_3 = b_3 + \sigma_2 \frac{a_2 b_2}{2a_1}, \] (4.28)

\[ m'_c = m_c + \frac{a_2^2}{4a_1 b_3}. \] (4.29)

This is Airy’s differential equation, and the general solution can be written as a linear combination of \(\text{Ai}(\zeta')\) and \(\text{Bi}(\zeta')\), where

\[ \zeta' = -\left(\frac{b'_3}{a_1}\right)^{1/3}(m - m'_c). \] (4.30)

We can now assess the validity of our approximation for \(y(m)\). First, let us ask for the order of \(\dot{y}\) relative to \(y\). From the known behavior of the Airy functions, this is \(J^{-1/3}\) in the failure zone \(\Delta m \leq J^{1/3}\), and of order \((\Delta m/J)^{1/2}\) in the overlap zone \(J^\eta \gg \Delta m \gg J^{1/3}\). We thus see that the higher order terms in Eqs. (4.12)–(4.14) are indeed smaller than those retained. In the same way the terms dropped in the differential equation for \(z(m)\) can be seen to be small. Second, the \(d^3y/dm^3\) term which was neglected in the differential equation (4.6) is of order \((\Delta m)^{3/2}/J^{1/2}\) in the overlap zone. Since \(\eta < 1\), this term is smaller than the \(\ddot{y}\) term, and higher order derivatives are smaller still.

The next step is to match the solution (4.4) and (4.26) using the known asymptotic forms of the Airy functions Ai and Bi, onto the DPI forms for \(m < m_c\) and \(m > m_c\). The matching zones can be taken to be any regions in which \(J^\eta \gg \Delta m \gg J^{1/3}\), where \(1 > \eta > 1/3\). The leading behavior of the Airy functions is either an exponential or a sine or cosine of \((\Delta m)^{3/2}/J^{1/2}\). We can ensure that the term \(b_2(m - m_c)^2/4a_1\) in the exponential in Eq. (4.26) is inconsequential on both sides if we choose \(\Delta m \ll J^{1/2}\). Accordingly we take the matching zone as

\[ J^{1/2} \gg |m - m_c| \gg J^{1/3}, \] (4.31)

In this zone we can approximate \(y(m) \approx z(m)\), and also neglect the small corrections in Eqs. (4.28) and (4.29). This amounts to saying that

\[ C_m \approx e^{-\sigma_2 \kappa_c(m - m_c)}[c_1 \text{Ai}(\zeta) + c_2 \text{Bi}(\zeta)], \] (4.32)

where \(c_1\) and \(c_2\) are two arbitrary constants, and
\[ \zeta = - \left( \frac{b_3}{a_1} \right)^{1/3} (m - m_c). \quad (4.33) \]

Let us first match Eq. (4.32) to the DPI solutions for \( m < m_c \). In order to treat all four solutions at the same time, we rewrite Eq. (3.9) as

\[ \cos q(m) = \frac{-t_1(m) + \sigma_1 t_2^2(m) - 4 t_2(m) f(m)}{4 t_2(m)}, \quad (m < m_c) \quad (4.34) \]

where \( f(m) = w(m) - 2 t_2(m) - E \), and \( \sigma_1 = \pm 1 \). The wavevector \( q(m) \) thus depends on both \( \sigma_1 \) and \( \sigma_2 \), and hence, so does the velocity \( v(m) \). We do not bother to write down these forms explicitly, except to note that \( i \sigma_1 \sigma_2 v(m) \) is positive. The DPI solutions may therefore be written as

\[ C_m = \frac{A_{\sigma_1 \sigma_2}}{2 \sqrt{i \sigma_1 \sigma_2 v(m)}} \exp \frac{i}{2} \int_{m_c}^{m} q(m') dm', \quad (4.35) \]

where \( A_{\sigma_1 \sigma_2} \) is a real constant which is introduced as a notational aid in distinguishing the different cases. In the matching zone, it follows from Eqs. (4.34, (4.1), (4.21), and (1.7), that

\[ \begin{align*}
\cos q(m) &\approx \cosh \kappa_c + \alpha \sigma_1 (m_c - m)/J^{1/2}, \\
q(m) &\approx i \sigma_2 \kappa_c + i \sigma_1 \sigma_2 \frac{\alpha}{\sinh \kappa_c} (m_c - m)/J^{1/2}, \\
v(m) &\approx -8 i \alpha \sigma_1 \sigma_2 \sinh \kappa_c |t_{2c}| ((m_c - m)/J)^{1/2}. 
\end{align*} \quad (4.36) \]

(We have written \( |t_{2c}| \) instead of \( t_{2c} \), with a view to including the case \( t_1 < 0, t_2 < 0 \), which we shall consider later.) Therefore,

\[ C_m \approx \frac{A_{\sigma_1 \sigma_2}}{4 \sqrt{2 \alpha t_{2c}} \sinh \kappa_c} \left( \frac{m_c - m}{J} \right)^{-1/4} \exp \left[-\sigma_2 \kappa_c (m - m_c) + \frac{2 \alpha \sigma_1 \sigma_2 (m_c - m)^{3/2}}{3 \sinh \kappa_c J^{1/2}} \right]. \quad (4.37) \]

Since \( \zeta \gg 1 \) for \( m < m_c \) in the zone (4.31), we may use the asymptotic forms [21]

\[ \begin{align*}
\text{Ai}(\zeta) &\approx \frac{1}{2 \sqrt{\pi}} \zeta^{-1/4} \exp \left( -\frac{2}{3} \zeta^{3/2} \right), \\
\text{Bi}(\zeta) &\approx \frac{1}{\sqrt{\pi}} e^{-1/4} \exp \left( \frac{2}{3} \zeta^{3/2} \right). 
\end{align*} \quad (4.38, 4.39) \]

Using Eq. (4.33) and comparing with Eq. (4.37), we see that we must use the function Ai when \( \sigma_2 = -\sigma_1 \), and Bi when \( \sigma_2 = \sigma_1 \). We can write

\[ C_m = KA_{\sigma_1 \sigma_2} e^{-\sigma_2 \kappa_c (m - m_c)} \times \begin{cases} 
\text{Bi}(\zeta), & \sigma_2 = \sigma_1; \\
2\text{Ai}(\zeta), & \sigma_2 = -\sigma_1,
\end{cases} \quad (4.40) \]

with
\[
K = \frac{\sqrt{\pi}}{4\sqrt{2}\alpha t_c \sinh \kappa_c} \left(\frac{a_1}{b_3}\right)^{-1/12} j^{1/4}
\]  

(4.41)

To connect Eq. (4.40) with the DPI solutions for \(m > m_c\), we make use of the reality principle, namely that the solution to the basic recursion relation (1.2) must be real for \(m > m_c\) if it is real for \(m < m_c\). Since the solutions to Eq. (3.3) now lead to complex \(q\), it is clear that we must add two DPI solutions in order to get a real result. To this end we define

\[
q_a(m) = i\sigma_2\kappa(m) + \chi(m), \quad m > m_c
\]

(4.42)

where \(\kappa(m)\) and \(\chi(m)\) are both real and positive, \(\kappa(m_c) = \kappa_c\), and

\[
\begin{align*}
\cosh \kappa \cos \chi &= -t_1/|t_2|, \\
\sinh \kappa \sin \chi &= (4t_2f - t_1^2)1/2/4|t_2|.
\end{align*}
\]

(4.43-4.44)

In terms of these quantities, we have

\[
\begin{align*}
\cos q_a(m) &= \cosh \kappa(m) \cos \chi(m) - i\sigma_2 \sinh \kappa(m) \sin \chi(m), \\
s_a(m) &\equiv -i\sigma_2 v_a(m) = 8|t_2(m)| \sinh \kappa(m) \sin \chi(m) \sin q_a(m).
\end{align*}
\]

(4.45-4.46)

[As before, we have written \(|t_2(m)|\) instead of \(t_2(m)\) with a view to subsequently including the case \(t_1 < 0, t_2 < 0\).] The corresponding quantities for the complex conjugate solution are given by \(q_b(m) = q_a^*(m)\), \(s_b(m) = s_a^*(m)\). The DPI solution into which Eq. (4.35) continues for \(m > m_c\) may therefore be written as

\[
C_m = \frac{1}{2} B_{\sigma_1\sigma_2} \left[ \frac{1}{\sqrt{s_a(m)}} \exp \left( i \int_{m_c}^m q_a(m')dm' + i\Delta_{\sigma_1\sigma_2} \right) + c.c. \right]
\]

(4.47)

where \(B_{\sigma_1\sigma_2}\) is real, \(\Delta_{\sigma_1\sigma_2}\) is a phase to be found, and c.c. denotes “complex conjugate”.

It remains to compare the asymptotic forms of Eqs. (4.40) and (4.47) in the overlap zone (4.33), and thus find \(\Delta_{\sigma_1\sigma_2}\) and the relation between \(A_{\sigma_1\sigma_2}\) and \(B_{\sigma_1\sigma_2}\). Using the asymptotic forms for \(A_i\) and \(B_i\), we have

\[
C_m \approx KA_{\sigma_1\sigma_2} \frac{e^{-\sigma_2\kappa_c(m-m_c)}}{\sqrt{\pi}} (-\zeta)^{-1/4} \times \begin{cases}
\cos \left[ \frac{2}{3}(-\zeta)^{3/2} + \frac{\pi}{4} \right], & \sigma_2 = \sigma_1; \\
2 \sin \left[ \frac{2}{3}(-\zeta)^{3/2} + \frac{\pi}{4} \right], & \sigma_2 = -\sigma_1.
\end{cases}
\]

(4.48)

To write Eq. (4.47) in a similar form, we first note that in the matching zone,

\[
\begin{align*}
q_a(m) &\approx i\sigma_2\kappa_c + \frac{\alpha}{\sinh \kappa_c}((m - m_c)/J)^{1/2}, \\
s_a(m) &\approx 8t_2\alpha \sinh \kappa_c \left(\frac{m - m_c}{J}\right)^{1/2} \exp \left[ i\sigma_2 \frac{\pi}{2} - i\sigma_2\alpha \frac{\cosh \kappa_c}{\sinh^2 \kappa_c} \left(\frac{m - m_c}{J}\right)^{1/2} \right].
\end{align*}
\]

(4.49-4.50)

Therefore,

\[
i \int_{m_c}^m q_a(m')dm' = -\sigma_2\kappa_c \Delta m + i\frac{2}{3}(-\zeta)^{3/2},
\]

(4.51)
where we have used Eqs. (4.20), (4.24), and (4.33) to simplify the term in \((-\zeta)^{3/2}\). Compared to this term, the correction proportional to \((\Delta m)^{1/2}\) in the exponent for \(s_a(m)\) is of higher order in \(1/J\) in the matching zone, and can be ignored. Doing this, and making use of Eqs. (4.33) and (4.41), we get

\[
C_m \approx \frac{K}{\sqrt{\pi} B_{\sigma_1 \sigma_2}} (-\zeta)^{-1/4} e^{-\sigma_2 \kappa_m \Delta m} \left[ \exp \left( i \frac{2}{3} (-\zeta)^{3/2} - i \frac{\pi \sigma_2}{4} + i \Delta_{\sigma_1 \sigma_2} \right) + \text{c.c.} \right].
\]  
(4.52)

Comparing with Eq. (4.48), we see that \(B_{\sigma_1 \sigma_2} = A_{\sigma_1 \sigma_2}/2\), while \(B_{\sigma_1, -\sigma_1} = A_{\sigma_1, -\sigma_1}\). Further, \(\Delta_{\sigma_1 \sigma_2}\) vanishes if \(\sigma_1 = -1\), and equals \(\pm \pi/2\) if \(\pm \sigma_2 = \sigma_1 = 1\). These results can be summarized as

\[
B_{\sigma_1 \sigma_2} = \frac{2 - \delta_{\sigma_1 \sigma_2}}{2} A_{\sigma_1 \sigma_2},
\]

(4.53)

\[
\Delta_{\sigma_1 \sigma_2} = \frac{\pi}{4} (1 + \sigma_1) \sigma_2.
\]

(4.54)

Putting together Eqs. (4.33), (4.47), (4.53), and (4.54), the connection formula may be written in the final form

\[
\frac{A_{\sigma_1 \sigma_2}}{2 \sqrt{i \sigma_1 \sigma_2 v(m)}} \exp \int_{m_c}^m q'(m') dm' \leftrightarrow C_m
\]

\[
\rightarrow \left( 1 - \frac{1}{2} \delta_{\sigma_1 \sigma_2} \right) A_{\sigma_1 \sigma_2} \left[ \frac{1}{\sqrt{s_a(m)}} \exp \left( i \int_{m_c}^m q_a(m') dm' + i \frac{\pi}{4} (1 + \sigma_1) \sigma_2 \right) + \text{c.c.} \right].
\]  
(4.55)

The wavevectors \(q\) and \(q_a\), and the velocity and speed, \(v(m)\) and \(s_a\), to be used for a given set of signs \((\sigma_1, \sigma_2)\) are given by Eqs. (4.36) and (4.49).

We use the double arrow notation \(\leftrightarrow\) advocated by Heading [22] and Dingle [23] to emphasize the bidirectionality of the connection formula. We refer readers to these authors for lucid discussions of this point, but since even as masterly and authoratitive a text as Landau and Lifshitz [24] states that connection formulas may only be used in one direction, it may be worth paraphrasing their remarks briefly. Thus, as stated by Heading, the notation means that there is a solution \(C_m\) to the recursion relation (1.2) with the stated asymptotic behaviors for \(m < m_c\) and \(m > m_c\). And, as stressed by Dingle, the formula merely states that a certain exponentially growing on one side of the turning point, which is free from the growing component, goes over into a certain oscillatory solution (with an exponentially growing envelope) on the other side, and vice versa. Likewise for the growing component. It says nothing about whether or not we can use the formula in both directions in physical problems where we do not have complete information. If, e.g., a solution with \(\sigma_1 = \sigma_2 = -1\) for \(m < m_c\) contains an admixture of the \(\sigma_1 = -\sigma_2 = 1\) solution of small but indeterminable magnitude, then we can say nothing about the amplitude or the phase of the oscillatory factor for \(m > m_c\). It is in these situations, where information is incomplete, that the reservations about the unidirectionality of the connection formulas are relevant.

The connection formula for the case where \(t_1 < 0\) and \(t_2 < 0\) can be derived in exact parallel by making minor modifications to the intermediate steps. The final form is sufficiently different to be worth giving separately:
\[ \frac{A_{\sigma_1\sigma_2}e^{i\pi m_c}}{2\sqrt{i\sigma_1\sigma_2 v(m)}} \exp i \int_{m_c}^m q(m')dm' \leftarrow C_m \]

\[ \rightarrow \left(1 - \frac{1}{2}\delta_{\sigma_1\sigma_2}\right) A_{\sigma_1\sigma_2} \left[ \frac{e^{i\pi m_c}}{\sqrt{s_a(m)}} \exp \left(i \int_{m_c}^m q_a(m')dm' - \frac{\pi}{4}(1 - \sigma_1\sigma_2)\right) + \text{c.c.} \right]. \quad (4.56) \]

The quantities \( v(m) \) and \( s_a(m) \) are given by the same formal expressions as before, but now

\[ q(m) \approx \pi + i\sigma_2\kappa_c + \frac{\alpha}{\sinh \kappa_c}((m_c - m)/J)^{1/2}, \quad (4.57) \]

\[ q_a(m) = \pi + i\sigma_2\kappa(m) + \chi(m). \quad (4.58) \]

In Eq. \((4.58)\), \( \kappa(m) \) and \( \chi(m) \) are also given by the same formal expressions as before, i.e., Eqs. (4.43) and (4.44).

**ACKNOWLEDGMENTS**

This work is supported by the NSF via grant number DMR-9616749. I am indebted to Wolfgang Wernsdorfer and Jacques Villain for useful discussions and correspondence about Fe\(_8\).

**APPENDIX A: WIDTH OF FAILURE ZONE OF DPI APPROXIMATION**

We have seen in Sec. 1 that the DPI approximation is valid everywhere except near turning points. Let us now estimate the size of the region where it fails. Suppose that \( q = 0 \) or \( \pi \) at the turning point, \( m_c \). As shown in Eqs. (3.14) and (3.15), \( q(m) \) and \( v(m) \) both vary as \( [(m - m_c)/J]^{1/2} \) for \( m \) near \( m_c \). Thus \( \dot{q} \sim (m - m_c)^{-3/2}J^{-1/2} \), and the first term in \( \Phi_2 \) is of order \( [(m - m_c)/J]^{-1/2} \). Next, note that \( r \sim [J/(m - m_c)]^{1/2} \), so that the second and third terms are both of order \( J^{1/2}(m - m_c)^{-3/2} \). The first term is subdominant to these two, and therefore, the condition that \( \Phi_2 \ll 1 \) reduces to

\[ |m - m_c| \gg J^{1/3}. \quad (A1) \]

In the case where the second factor in \( v(m) \) vanishes, we have \( t_1 + 4t_2 \cos q \sim [(m - m_c)/J]^{1/2} \), and \( q - q_e \sim [(m - m_c)/J]^{1/2} \). Thus the integrand of the first term in \( \Phi_2 \) varies as \( 1/(m - m_c)^2 \), and the term itself is of order \( 1/(m - m_c) \). However, \( r \sim [J/(m - m_c)]^{1/2} \) as before, so that the second and third terms are again of order \( J^{1/2}(m - m_c)^{-3/2} \), and much greater than the first term. The condition for validity of the DPI form is again given by Eq. (A1).

The condition can be written in alternative form by noting that near the region of failure, \( r(m) \sim 1/v(m) \), and that \( \dot{v} \sim \dot{q} \). Thus \( dr/dm \sim \dot{q}/v^2 \), and the last term in \( \Phi_2 \) can also be shown to be of order \( \dot{q}/v^2 \). Thus the condition for validity can be written as

\[ \dot{q}(m) \ll v^2(m). \quad (A2) \]
REFERENCES

* Electronic address: agarg@nwu.edu

[1] R. B. Dingle and J. Morgan, Appl. Sci. Res. 18, 221 (1967); ibid. 18, 238 (1967).
[2] K. Schulten and R. G. Gordon, J. Math. Phys. 16, 1971 (1975).
[3] P. A. Braun, Rev. Mod. Phys. 65, 115 (1993).
[4] P. A. Braun, Teor. Mat. Fizika 37, 355 (1978) [Sov. Phys. Theor. Math. Phys. 37, 1070 (1978)].
[5] J. L. van Hemmen and A. Sütő, (a) Europhys. Lett. 1, 481 (1986); (b) Physica 141B, 37 (1986).
[6] C. Sangregorio, T. Ohm, C. Paulsen, R. Sessoli, and D. Gatteschi, Phys. Rev. Lett. 78, 4645 (1997).
[7] A.-L. Barra, P. Debrunner, D. Gatteschi, Ch. E. Schultz, and R. Sessoli, Europhys. Lett. 35, 133 (1996).
[8] R. Caciuffo, G. Amoretti, A. Murani, R. Sessoli, A. Caneschi, and D. Gatteschi, Phys. Rev. Lett. 81, 4744 (1998).
[9] M. V. Berry and M. Wilkinson, Proc. Roy. Soc. Lond. A 392, 15 (1984).
[10] A. Garg, Europhys. Lett. 22, 205 (1993).
[11] A. Garg, submitted to Europhysics Letters.
[12] J. Villain and Anna Fort, submitted to Europhys. B.
[13] W. Wernsdorfer and R. Sessoli, Science 284, 133 (1999).
[14] A. Garg, Phys. Rev. B 51, 15161 (1995).
[15] A. Garg, Phys. Rev. Lett. 83, 4385 (1999); and submitted to Phys. Rev. B.
[16] There are clearly situations where it is better for $m$ to take on non-integer values, or to change in increments other than unity. For developing the formalism, however, little is gained by incorporating these refinements, and it is sufficient to let $m$ take on contiguous integer values.
[17] Note that it is possible for more than one pair of $q$’s to coalesce at a turning point, as in all cases with the letter symbol $B$. For non-Hermitean problems, turning points are still characterized by the coalescence of two roots for $q$, but the directions in which they approach or separate can be arbitrary.
[18] M. V. Berry and K. E. Mount, Rep. Prog. Phys. 35, 315 (1972).
[19] A. Garg, J. Math. Phys. 39, 5166 (1998).
[20] David Bohm, Quantum Theory (Prentice-Hall, Englewood Cliffs, 1951), Chap. 12.
[21] Handbook of Mathematical Functions, M. Abramowitz and I. A. Stegun, eds. (Dover, New York, 1970), Sec. 10.4.
[22] J. Heading, An Introduction to Phase-Integral Methods (Methuen, London, 1962). See Chap. 1, Sec. 1.6 in particular.
[23] R. B. Dingle, Asymptotic Expansions: Their Derivation and Interpretation (Academic Press, London, 1973). See Chap. XIII, Secs. 13.3 and 13.4 in particular.
[24] L. D. Landau and E. M. Lifshitz, Quantum Mechanics (Pergamon, New York, 1977), 3rd ed. See Sec. 47.
FIGURES

FIG. 1. Schematic band energy curves arising from five term recursion relations. Curve 1 arises if $|t_1/4t_2| > 1$, curve 2 if $-1 < t_1/4t_2 < 0$, and curve 3 if $0 < t_1/4t_2 < 1$. The dual labelling scheme for the critical energies $U_0$, $U_\pi$, etc. is shown.

FIG. 2. Critical energy curves in the case where $-t_1(m)/4t_2(m) < -1$ for all $m$. The points $m = m_b$ and $m = m_c$ are turning points of type $A$ and $A$, respectively, for the energy $E$.

FIG. 3. Same as figure 2, but with $-t_1(m)/4t_2(m) \in [-1, 1]$ for some $m$. These critical curves arise from the Hamiltonian (1.1) for Fe$_8$. Note that $U_s$ is the lower band edge $U_-$ for the central $m$ region, and the forbidden critical energy $U_f$ for the outer $m$ regions. Correspondingly, $U_0$ is the internal critical energy $U_i$ in the central region, and the lower band edge $U_-$ in the outer regions. The point $m = m_c$ is a type $A'$ turning point for the energy $E$.

FIG. 4. Magnified view of lower left hand portion of Fig. 3. The points $m = m_t$ and $m_c$ are turning points of type $A$ and $B$ respectively.

FIG. 5. Band energy curves in the vicinity of a type $A'$ turning point.

FIG. 6. Possible band energy curve for a recursion relation with seven or more terms.

FIG. 7. Critical curves for a system with band energy curves as shown in Fig. 3.
$U(m)$

$E$

$m_b$

$m_c$

$U_+(m)$

$U_-(m)$

$U_*(m)$
$U_\pi = U_+$

$U_0 = U_i$

$U_0 = U_-$

$U_\star = U_*$

$U_\star = U_*$

$m^*$

$m_c$

$m$
\[ U_0 = U_i \]

\[ U_* = U_f \]

\[ m_t \]

\[ m_c \]

\[ m^* \]
$m_a < m$
