Chirped Random Mirrors and Adiabatic Matrix Products

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Abstract

A variety of physical problems benefit from the possibility of analytic calculation of products of large numbers of slowly varying matrices. These problems include chirped dielectric mirrors, random chirped dielectric mirrors, Rydberg atoms etc. We derive the matrices specific to chirped and random chirped dielectric mirrors and discuss methods for analytic understanding of the product. We first show that an approximation very similar to the well-known adiabatic approximation, and corrections thereto, can be applied to such products “most places” – specifically where all the eigenvalues of the matrices are sufficiently different relative to the rate of change of the eigenvectors. However, we show that this condition is generically violated when physical behavior changes radically e.g. at the band edge in the dielectric mirror or the turning point of a discrete version of the Schrodinger equation. We present progress towards analytic approximations of such matrix products in this limit.
Objectives

This senior project report has two objectives: first to relate the properties of chirped mirrors and random chirped mirrors to the product of a large number of slowly varying matrices and second to analyze such products of slowly varying matrices in terms of an adiabatic approximation. A large class of problems can be formulated as a product of a large number of slowly varying matrices. These include recursion relations or difference equations which have appreciable physical interest, such as models of Rydberg atoms, transfer matrix formulations of non-random and random chirped dielectric mirrors, discrete approximations to differential equations, each with slowly changing coefficients. Significant work has already been done in all of these fields. This project was first intended to address simply the problem of the chirped, random dielectric mirror: to use the transfer matrix formulation, which seems to be relatively infrequently applied analytically to this problem, to analyze the behaviors and to provide simple analytic results to facilitate engineering of such mirrors. During this investigation, we were unable to find prior work on the adiabatic approximation for matrices that dealt satisfactorily with a situation of specific interest to mirrors: the region in which there is a change from propagating to evanescent waves. Moreover, we believe that other fields, such as the Rydberg atom problem, have also not appropriately treated such regions. Thus such a treatment became an additional objective of the project.

I. INTRODUCTION

There are a large number of physical situations the properties of which are easily and effectively described in terms of products of large numbers of matrices. An archetypal situation of continuing interest is the dielectric mirror, which consists of a large number of bilayers of materials with different optical properties. Successive small reflections from such bilayers can add coherently to result in nearly perfect reflection from the mirror. This problem can be addressed by relating the optical fields on either side of a bilayer through a matrix, typically called the transfer matrix. The matrix describing the entire system can then be expressed as

\[ T_N = \left( \prod_{j=0}^{N-1} T_j \right) \]  

(1)
with the product of the matrices chosen such that a matrix with a larger value for the index $j$ is to the left of a matrix with a small index. For systems with some randomness, it is also possible to calculate various averages of various properties in terms of transfer matrices: typically transfer matrices with larger dimensions [1]. This is of specific interest as it is a technique being developed locally by the CLips NSF Science and Technology Center for making such dielectric mirrors [4]. This technique is attractive as it is relatively cheap but is of concern as it results in relatively large randomness. Hence a clear method for modeling the importance of such randomness is important.

A simple dielectric mirror with constant properties of the bilayers results in reflection only for a typically quite narrow band of wavelengths called the “band gap”. This band gap is typically centered around the region in which the width of the bilayer is a half integer number of wavelengths and its fractional width is proportional to $|n_1 - n_2| / (n_1 + n_2)$ where $n_1$, $n_2$ are the refractive indices of the two different layers in a bilayer. The results for a simple constant bilayer mirror are easy to derive in terms of eigenvalues of the relevant transfer matrices. However, it is commonly interesting to consider more complicated mirrors for which properties of the bilayers change slowly with the index of the layers: these are typically referred to as “chirped” dielectric mirrors. Such chipped mirrors can have reflections over a wider range of wavelengths, and also to have different phase delays on reflection for different wavelengths [6]. For specific physical applications such as ultrafast lasers, such engineer such phase delays can be valuable. Approximate methods need to be used in this case, and we suggest on improvements to present methods for such mirrors below.

In addition, a number of problems, such as the properties of Rydberg atoms [3], can be expressed in terms of an ordinary linear first order difference equation such as

$$\phi_{j+M} = \sum_{k=0}^{M-1} a(k, j) \phi_{j+k}$$

(2)

where the are $\phi_j$ are a sequence of numbers or vectors dependent on an index $j$, and all $\phi$’s are from (for example) from $\phi_j$, $j = 0, 1, \ldots M - 1$. It is easy to see that all such difference equations - whether $\phi$ can be related to such matrix products, with matrices that vary slowly provided that the coefficients of the difference equation vary slowly. It is also (usually) possible to reduce matrix products to the solution of difference equations, typically in many ways. Provided that the elements of the matrices and/or the resultant coefficients of the difference equation change slowly with index and provided that the equation can be
transformed in this way, such difference equations can be approximated, often in many ways, by differential equations. The difference equation relevant to Rydberg atoms has also been analyzed with the difference operator given as the exponential of the derivative (or quantum mechanical momentum) operator and then analyzed within the context of a Hamiltonian depending on the position and momentum.

Such tactics have been employed in various aspects of the literature, and known approximations such as (or related to) WKB approximations have been used [3, 9]. Here we suggest that it is more direct, more reliable and more productive to consider the equations as matrix equations e.g. in the form of and then to make an adiabatic approximation on this matrix product. In effect, this technique assumes that the matrices $T_j$ are slowly varying almost everywhere or (more precisely) that the $T_j$ are almost always diagonalizable and that the basis in which they are diagonal is slowly varying almost everywhere. This technique is not only more direct by also allows the solution of a variety of equations that cannot be solved by these other techniques. Moreover, it is more “algorithmic”, requiring less thought and/or experimentation with the problem. It more naturally gives a precise meaning to the term “slowly varying”, which can depend on the choice of variables in the difference equation approach and, in the matrix formulation can be made more precise and independent of the way in which the problem is expressed. Finally, it is more easily extendable to a slightly wider range of problems e.g. those in which the matrix (or coefficients) change slowly as a function of most places but change abruptly some places.

The adiabatic approximation for time-continuous propagation has been known since the very early days of quantum mechanics. Here is is proven that, provided the Hamiltonian changes slowly - roughly provided that the basis in which the Hamiltonian is diagonal changes slowly in the time scale given by the differences between energy eigenvalues - then the probability that the system is in a given state does not change and the phase of that state is given by the integral of the phase change associated with the time-averaged energy of that state. It seems to be much less well appreciated that discrete products of slowly varying matrices can also be approximated in a very similar fashion. Roughly, it is expected that such matrix products can be of eqn 1 can be written approximately as

$$T_N \approx S_{N-1} \left( \prod_{j=0}^{N-1} \Lambda_j \right) S_0^{-1}$$

(3)

where the $S_j$ are similarity transformations so that the diagonal matrix $\Lambda_j = S_j^{-1}T_jS_j$. 

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Clearly, if there are specific values of \( j j = k_1, k_2, \ldots, k_K \) for which the basis changes quickly, then this product can be written as

\[
T_N \approx \prod_{l=1}^{K} \left[ S_{k_l} \left( \prod_{j=1}^{N-1} \Lambda_j \right) S_{k_{l-1}}^{-1} \right]
\]  

(4)

with \( k_0 = 0 \) and \( k_{K+1} = N - 1 \). Clearly it is not a requirement that these matrices have any relationships symmetry, Hermiticity, unitarity or similar, however, they must be diagonalizable most places: at least our discussion will assume this. For many such matrix formulations for difference equations that approximate differential equations, it can be shown (and is argued below) that the adiabatic approximation for the matrix formulation corresponds to the WKB approximation or, more broadly, to approximations based on the principle of asymptotic balance on the Ricatti transformation for such differential equations.

In what follows we will discuss a general adiabatic approximation for such matrix products. We also give criteria for these approximations to be valid and ways to calculate corrections. We note that there are places where the simple adiabatic approximations given above fail in “generic” ways, at places we will call turning points. Such generic failures can be understood by thinking about classical turning points in the Schrödinger equation, or, more rather, in a difference equation that approximates the Schrödinger equation near such a turning point. At such points the nature of the physics changes abruptly, typically from propagating to evanescent solutions. Such points are of broad physical interest: they are important to the states of Rydberg atoms and also correspond to having the local bandgap of a chirped mirror equal to the frequency of the incident light, which is expected to happen for all light that is efficiently reflected by such a mirror. Exactly as the adiabatic approximation is equivalent to the WKB approximation for the corresponding differential equation, the behavior of the product of matrices near such generic points is argued below to be analogous to the behavior of the Schrödinger equation near a turning point. Such turning points seem not to have been previously addressed with similar accuracy in previous works on difference equations. When completed, such work will allow more precise determination of the properties of systems with such turning points.

This paper is organized as follows. The next section reviews the formulation of transfer matrices for dielectric mirrors, and the nature of the eigenvalues and eigenvectors of these matrices. The third section expands this discussion to random dielectric mirrors. The fourth section discusses the discrete adiabatic approximation and relevant choices for the similarity
transformations required to perform this approximation. The fifth section discusses turning points, and how these can be better treated in the matrix approximation. Our conclusions are given in the final section.

II. CHIRPED DIELECTRIC MIRRORS

A theoretical investigation of dielectric mirrors serves not only as a starting point and motivation for the following and more general analysis, but as a prototypical example of a class of problem that may benefit from each aspect of that analysis. Traditionally, theoretical descriptions of the optical behavior of dielectric mirrors are made by use of transfer matrices [5]. Transfer matrix formulations are well-suited to the modeling of transport through an approximately stratified medium. The propagation of light through dielectric mirrors, exactly stratified by definition, is no exception. The details of this particular transfer matrix formulation and an introduction to its analysis follows.

The propagation of light through the entirety of a dielectric mirror may be understood by first modeling the transmission and reflection of light incident upon a single bi-layer. Considering both left-ward and right-ward moving waves, the propagation of light of wavelength $\lambda$ through the bi-layer is represented by the product of four matrices

$$ T = D^l P^l D^r P^r $$

$$ = \begin{pmatrix}
\frac{1}{2} (1 + \frac{n_l}{n_r}) & \frac{1}{2} (1 - \frac{n_l}{n_r}) \\
\frac{1}{2} (1 - \frac{n_l}{n_r}) & \frac{1}{2} (1 + \frac{n_l}{n_r})
\end{pmatrix}
\begin{pmatrix}
e^{i\frac{2\pi n_l}{\lambda} d} & 0 \\
0 & e^{-i\frac{2\pi n_l}{\lambda} d}
\end{pmatrix}
\begin{pmatrix}
\frac{1}{2} (1 + \frac{n_r}{n_l}) & \frac{1}{2} (1 - \frac{n_r}{n_l}) \\
\frac{1}{2} (1 - \frac{n_r}{n_l}) & \frac{1}{2} (1 + \frac{n_r}{n_l})
\end{pmatrix}
\begin{pmatrix}
e^{i\frac{2\pi n_r}{\lambda} d} & 0 \\
0 & e^{-i\frac{2\pi n_r}{\lambda} d}
\end{pmatrix}
$$

corresponding respectively to Fresnel reflection due to the change of index at the left of bi-layer, wave propagation in the left layer with index $n_l$, Fresnel reflection due to the change of index in the middle of the bi-layer, and wave propagation in the right layer with index $n_r$.

This transfer matrix describes the transport of phasor representations of left- and rightward moving waves from the right side of $j$th bi-layer to the left:

$$ \begin{pmatrix}
v_{j+1}^{\text{left}} \\
v_{j+1}^{\text{right}}
\end{pmatrix} = v_{j+1} = T_j v_j = \frac{1}{1 - a^2}
\begin{pmatrix}
e^{2ik_n} - a^2 e^{2iak_n} & a(e^{-2ik_n} - e^{-2iak_n}) \\
a(e^{2ik_n} - e^{-2iak_n}) & e^{-2ik_n} - a^2 e^{-2iak_n}
\end{pmatrix}
\begin{pmatrix}
v_j^{\text{left}} \\
v_j^{\text{right}}
\end{pmatrix} $$

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where \( n = \frac{n_l + n_r}{2} \) is the average index, \( a = \frac{n_r - n_l}{n_r + n_l} \) is the measure of the difference in the indices, and \( k_j = \frac{2\pi d_j}{\lambda} \) is the wavevector per cell. It should be noted that the above derivation of the bi-layer transfer matrix makes a design assumption, the physical length \( d_j \) of the two sub-layers of the \( j \)th bi-layer is the same. A perhaps more traditional alternative would be to design the mirror such that the phase change imparted by each layer is the same, i.e. the optical lengths are equal: \( \phi \lambda = 2\pi d_l n_l = 2\pi d_r n_r \). Under this design, the transfer matrix has a slightly different form:

\[
T_j = \frac{1}{1 - a^2} \begin{pmatrix}
e^{2ik_jn} - a^2 & a(e^{-2ik_jn} - 1) \\
a(e^{2ik_jn} - 1) & e^{-2ik_jn} - a^2
\end{pmatrix}
(7)
\]

Once the optical behavior of a single bi-layer has been represented by a transfer matrix, the corresponding representation for that of the full mirror is readily determined. The transport of left- and right-ward moving waves from the right side of the mirror to left is determined by a matrix product

\[
v_N = T_{N-1}v_{N-1} = T_{N-1}T_{N-2}v_{N-2} = ... = T_{N-1}...T_0v_0 = \mathcal{T}_N = (\prod_{j=0}^{N-1} T_j)v_0 = \mathcal{T}v_0
(8)
\]

So the product \( \mathcal{T} \) is the transfer matrix for the full mirror. For a chirped mirror, the transfer matrices, \( T_j \), component in this product, are slowly varying, and thus a good understanding of such slow varying, i.e. adiabatic, matrix products becomes our goal. As is detailed in the more general discussion of the fourth section, an analysis of the behavior of the eigenvectors and eigenvalues of the transfer matrices, \( T_j \), component in this product, i.e. how these change with the parameter \( k_j \), is necessary. We find, in particular, that for the matrix of equation 7 that the eigenvalues always have unit product and are either complex conjugates on the unit circle or real, with one greater than unity and one less than than unity.

We note that at points where the eigenvalues are \( \pm 1 \) that both eigenvalues are degenerately \( \pm 1 \) and that the matrix can not be diagonalized but has a more general Jordan normal form. We note that, as this matrix is \( \textit{not} \) unitary or Hermitian, there is no constraint that the eigenvalues should not be “generically” the same. Such behavior, in fact, is expected generically for un-constrained matrices, whenever the determinental equation for the eigenvalues has a double root. Moreover, it is the case that in the region surrounding a point
where this condition is satisfied, the eigenvalues and eigenvectors both have square-root singularities, and there is an abrupt change in the similarity transformation that diagonalizes this matrix at these points. Here, then is a situation where although the transfer matrix is slowly varying, the eigenvectors are not. This suggests a critical change in behavior, and in the physical context of the dielectric mirror we identify these points as those at which light stops propagating and becomes evanescent, the band-gap edge. Analysis in such regions, both in the context of this specific problem and more generally, requires a good deal of care, as will be discussed below.

III. RANDOM CHIRPED DIELECTRIC MIRRORS

The above modeling and analysis of dielectric mirrors is limited in its assumption that the mirrors are perfectly constructed. Real-world manufacturing processes, however, will not be perfect: these will introduce disorder in the mirrors, a random variation in the layer thicknesses e.g. We are particularly motivated to understand the optical behavior of disordered mirrors given that the manufacturing technique being developed at CLiPS [4] would introduce a significant amount of exactly this type of randomness. We, as a first step, are interested in the average behavior of an ensemble of mirrors that are produced by such a process. We note that this is not, as may be naively expected, to be found by simply applying the above analysis to the dielectric mirror of average layer thicknesses nor by averaging individually the transfer matrix for each bi-layer and proceeding as before. The first “average” is misleading and mathematically incorrect, as the dependence of transfer matrix product, and thus of the reflective behavior of the mirror, on layer thicknesses is non-linear. The average transfer matrix resulting from the second approach, while mathematically accurate given statistical independence of the bi-layers, is of little interest: the averaged elements of the transfer matrix are not quantities that give directly meaningful physical interpretations in the context of the reflective quality of the mirror.

Previous work [2], following a general technique developed for the theoretical study of 1-D wave transport in disordered systems [1], investigated in the same context the average behavior random traditional mirrors, mirrors with constant average layer thickness. We follow here the same technique, which generalizes the transfer matrix, establishing in particular that the symmetric direct product of transfer matrices themselves satisfy the properties of
transfer matrices, and further include as terms the quantities whose averages are of direct interest. Specifically, the average behavior of a chirped, random dielectric mirror can be determined by taking the average of the product symmetric direct products of the transfer matrices for each bi-layer,

$$T^{(2)} = \prod_j \{T_j \otimes T_j\}_{\text{Sym}}$$  \hspace{1cm} (9)

where \(\{\otimes\}_{\text{Sym}}\) gives the symmetrized direct product of the matrices and the bar indicates the average. This averaged generalized full transfer matrix, assuming statistical independence of each term, i.e. bi-layer, is equivalently given by the product of averaged symmetric direct products,

$$T^{(2)} = \prod_j \{T_j \otimes T_j\}_{\text{Sym}}$$  \hspace{1cm} (10)

where

$$T_j^{(2)} = \{T_j \otimes T_j\}_{\text{Sym}} = \{D^{rl} \otimes D^{rl}\}_{\text{Sym}} \{P^{rl}_j \otimes P^{rl}_j\}_{\text{Sym}} \{D^{lr} \otimes D^{lr}\}_{\text{Sym}} \{P^{lr}_j \otimes P^{lr}_j\}_{\text{Sym}}$$  \hspace{1cm} (11)

Assuming a Gaussian distribution for wavevector with mean \(k\) and standard deviation \(-\frac{1}{2n} \ln(s + 1)\), where \(s\) is a measure of disorder, the average symmetric direct product of the propagator matrices takes the form

$$\{P^{\alpha}_j \otimes P^{\alpha}_j\}_{\text{Sym}} = \begin{pmatrix} (1 - s)e^{2ikn} & 0 & 0 \\ 0 & 1 & 0 \\ 0 & 0 & (1 - s)e^{-2ikn} \end{pmatrix}$$  \hspace{1cm} (12)

and the now 3-by-3 transfer matrix is

$$T_j^{(2)} = \frac{1}{(1 - a^2)^2} \begin{pmatrix} (1 - s)((1 - s)(a^2 + e^{4ikn}) - 2a^2e^{2ikn}) & -2a^2e^{-2ikn}((1 - s)(a^2 + e^{4ikn}) - (a^2 + 1)^2 - 4a^2cos(2kn)(1 - s) \\ a(1 - s)((1 - s)(a^2 + e^{4ikn}) - (a^2 + 1)e^{2ikn}) & (a^2 + 1)^2 - 4a^2cos(2kn)(1 - s) \\ 2a^2e^{2ikn}(1 - s)((1 - s)cos(2kn) - 1) & -2a^2e^{-2ikn}((1 - s)(a^2 + e^{-4ikn}) - (a^2 + 1) \end{pmatrix}$$  \hspace{1cm} (13)

As before, we discuss the eigenvalues and eigenvectors of this transfer matrix generically. It is easy to see that one eigenvalue is always along the real axis and has magnitude greater than unity. This eigenvalue is roughly the eigenvalue that corresponds to the scattering behavior of the system or is dominant in the calculation of the average transmittance over
long distances: it is exactly unity in the absence of disorder. The other two eigenvalues are either complex conjugates or are both real, and describe scattering and propagation over shorter distances, roughly propagation over distance. When this pair of eigenvalues are complex conjugates, both have magnitude less than unity. When all are real, one is greater than unity, one has magnitude less than unity, and the last one has magnitude in between these. There is generically a point at which this character of the eigenvalues changes from a pair of complex conjugate eigenvalues and one real eigenvalues to three real ones. This again is a region in which extra care must be taken.

IV. ADIABATIC APPROXIMATION

The primary objective of this paper is to discuss methods for computing the product of a large number of matrices that vary slowly with an index, specifically

$$T_N = \left( \prod_{j=0}^{N-1} T_j \right)$$  \hspace{1cm} (14)

where the $T_j$ are arbitrary $n \times n$ square matrices that are (almost everywhere) assumed to vary slowly as with changing $j$ and here (and below) all matrix products written with a product sign $\prod$ are assumed to be “time” ordered, which is to say that matrices with lower index $j$ are to the right of matrices with higher index $j$. We further assume that $T_j$ can be diagonalized for almost all $j$. Moreover, we will assume that for almost all $j$, all the eigenvalues of $T_j$ are distinct. Generalizing to the case that $T_j$ has degenerate eigenvalues or a more complicated Jordan normal form for large ranges of $j$ is beyond the scope of this paper: in some instances, this is a simple extension of our techniques, in others it is exceedingly difficult. Other than these constraints we put no restrictions on these matrices.

In understanding this product, it will be useful to consider the propagation of vector $\phi$. Specifically starting from an initial vector $\phi_0$ we can recursively calculate

$$\phi_{j+1} = T_j \phi_j$$  \hspace{1cm} (15)

or equivalently

$$\phi_k = \left( \prod_{j=0}^{k-1} T_j \right) \phi_0 = T_k \phi_0$$ \hspace{1cm} (16)
We note that this equation makes it clear that the matrix $T_j$ can be thought of as the coefficients of a set of $n$ coupled first order linear difference equations. Thus our discussion below can also be thought of as applying to most coupled linear first order difference equations, provided that the coefficients of these difference equations vary slowly. It is also generally possible, often in many ways, to relate higher order linear difference equations to first order difference equations with more variables. Thus, provided that this can be done in at least one way that results in slowly varying $T_j$ that can usually be diagonalized, our discussion also applies to such equations.

Our first step in computing this product will be to diagonalize or make an eigenvalue decomposition of $T_j$. Assuming that the eigenvalues are not degenerate, there are $n$ continuous free parameters in the choice of the similarity matrix $S_j$ that accomplishes this diagonalization. For any similarity matrix $\tilde{S}_j$ and any non-singular diagonal matrix $D_j$ and provided that $S_j = D_j \tilde{S}_j$, we have that

$$T_j = \tilde{S}_j \Lambda_j \tilde{S}_j^{-1} = \tilde{S}_j D_j \Lambda_j D_j^{-1} \tilde{S}_j^{-1} = (S_j)\Lambda_j(S_j)^{-1}$$

(17)

where $\Lambda_j$ is the diagonal matrix of eigenvalues of $T_j$. In addition to these $n$ continuous degrees of freedom there are additional discrete degrees of freedom: specifically the columns of $S$ can be permuted in any way desired. Discussion of the errors in the techniques examined below are easier if we make appropriate choices for these discrete and continuous degrees of freedom. Specifically, it is desirable to make these choices so that the slow variation in $T_j$, insofar as possible, implies a slow variation in both $\Lambda_j$ and $S_j$. Permutation of the columns of $S_j$ permutes the diagonal elements of $\Lambda_j$: these permutation should be chosen in a natural way so that each diagonal matrix element and each column of $S$ changes as slowly as naturally possible. We will also insist that $\det(S_j) = 1$, and . Further useful constraints on $S_j$ are discussed below.

If we define $r_j = S_{j+1}^{-1}S_j$ and $R_j = \tilde{D}_j^{-1}r_j$, where $\tilde{D}_j$ is another arbitrary invertable diagonal matrix with unit determinant, which will be discussed more below and is assumed to be close to unity. The matrix product can be rewritten:

$$T_k = \prod_{j=0}^{k-1} S_j \Lambda_j S_j^{-1} = S_k(\prod_{j=0}^{k-1} (S_{j+1}^{-1}S_j)\Lambda_j)S_0^{-1} = S_k(\prod_{j=0}^{k-1} \tilde{D}_j R_j \Lambda_j)S_0^{-1}$$

(18)

As we are assuming that $S_j$ varies slowly with $j$, it is reasonable to expect that $R_j \approx 1$
e.g. is close to the identity matrix. Prior to putting constraints on $S$ and hence $R$, or discussing the value of the potential freedom associated with we examine what this means for approximation of the matrix product.

As we expect that in most regions $R_j$ will be close to identity, we are motivated to approximate the product remaining in 18 by analogy to the quantum mechanical technique known as time-dependent perturbation theory. Using this analogy to quantum mechanics, we first define a propagator for the unperturbed motion:

$$U^0_j = \prod_{j' = 0}^{j-1} \tilde{\Lambda}_{j'+1}$$

and write the perturbation $R_j$ in the interaction basis:

$$R^I_j = (U^0_j)^{-1} R_j U^0_j.$$  

Then the product takes the exact form

$$\mathcal{T}_k = S_{k-1} U^0_{k-1} \left( \prod_{j=1}^{k-2} R^I_j \right) \tilde{\Lambda}_1 R_0 \tilde{\Lambda}_0 S_0^{-1}.$$  

where the “interaction product”

$$\mathcal{T}^I_{k-1} = \prod_{j=1}^{k-2} R^I_j$$

remains to be determined.

The well known technique for dealing with this is to write $R^I_j = 1 + \delta R^I_j$ and then to expand in powers of $\delta R^I_j$ to find

$$\mathcal{T}^I_{k-1} = 1 + \sum_{j=1}^{k} \delta R^I_j + \sum_{1 \leq j < j' \leq k} \delta R^I_{j'} \delta R^I_j + \ldots.$$  

while the terms proportional to $\delta R$ are naively quite large and growing with increasing order for large $k$ even if $\delta R$ is small as the term containing $M$ powers of $\delta R^I_j$, it is important to note that in many circumstances this is not the case. First, the terms that we have already taken into account grow exponentially in $k$, so that any power, however large, seems a “small” change. More importantly, if $\delta R_j = R_j - 1$ is small and approximately constant, then unless ratios of the various $\Lambda_j$ are close to unity the off-diagonal terms of $\delta R^I_j$ will change dramatically over a range of $j$ with $\Delta_{j,\alpha,\beta} \approx | \ln (\Lambda_{j,\alpha}/\Lambda_{j,\beta}) |$, where $\alpha, \beta$ index the matrix
elements and the $\Lambda_{j,\alpha}$ are the eigenvalues corresponding to the off-diagonal term, $\delta R_{j,\alpha\beta}$ considered. Thus, we expect the off-diagonal terms of the first sum to have magnitude be approximately $\delta R_{j,\alpha\beta} \Delta j_{\alpha\beta}$. Here the value of $j$ needs to be chosen with some care. It will be both ends of any region if in which the magnitude of $\delta R_{j,\alpha\beta}$ has approximately constant magnitude but oscillates - this is to be expected when $\Lambda_{j,\alpha}/\Lambda_{j,\beta}$ is on the unit circle, but not close to unity. It is near the location where $\delta R_{j,\alpha\beta}$ is large if its magnitude changes rapidly, which is to be expected when $\Lambda_{\alpha}/\Lambda_{\beta}$ sufficiently far from the unit circle. In any case, these terms are not expected to be large in comparison to the on-diagonal terms. The diagonal terms of the first term and the on-diagonal terms of the second term will have approximate magnitude

$$k \left[ \delta R_{j,\alpha\alpha} + \delta R_{j',\alpha\beta} \delta R_{j,\beta\beta} \Delta j_{\alpha\beta} \right]$$

(24)

where these are ‘typical’ values. Here, we expect that these terms are, in fact, the first non-unity term in an expansion of $\exp (x)$, which term, when exponentiated, results only in a small change in the (logarithm) of the total product. Thus, it appears that the criterion for a “good” approximation is that $\delta R_{\alpha\alpha} \ll \Delta j_{\alpha\beta}$, $\delta R_{j',\alpha\beta} \delta R_{j,\beta\beta} \Delta j_{\alpha\beta} \ll \Delta j_{\alpha\beta}$.

With these considerations in mind, we examine our possible choices for $R_j$. We first define

$$W_j = S_j^{-1} T_{j+1} S_j$$

(25)

and note that $R$ diagonalizes $W$

$$R_j W_j R_j^{-1} = (D_j S_{j+1}^{-1} S_j)(S_j^{-1} T_{j+1} S_j)(S_j^{-1} S_{j+1} D_j^{-1}) = D_j S_{j+1}^{-1} T_{j+1} S_{j+1} D_j^{-1} = \Lambda_{j+1}$$

(26)

so

$$R_j W_j = \Lambda_{j+1} R_j$$

(27)

Supposing that $W_j = \Lambda_j + \delta W_j$, with $\delta W_j = S_j^{-1} (T_{j+1} - T_j) S_j$ expected to be small, we can estimate the off-diagonal matrix elements of $R_j$ by choosing the diagonal terms to be unity and solving 27 by perturbation theory to find

$$R_{j,\alpha\beta} = \delta W_{j,\alpha\beta} / (\Lambda_{j,\alpha} - \Lambda_{j,\beta})$$

(28)
with the error in this approximation being \( O \left( \delta W_{j,\alpha \beta} \delta W_{j,\beta \alpha} (\Lambda_{j,\alpha} - \Lambda_{j,\beta})^{-2} \right) \). In order to retain the constraint that \( \text{det} \left( R_j \right) = 1 \) we can then choose the diagonal terms to be

\[
R_{j,\alpha \alpha} = 1 + \sum_{\beta \neq \alpha} \delta W_{j,\beta \alpha} \delta W_{j,\alpha \beta} (\Lambda_{j,\beta} - \Lambda_{j,\alpha})^{-2}
\]  

(29)

we note that this makes the two terms in eqn 24 approximately equal. It is also makes clear the fact that the true criterion for the changes in \( T \) to be small is that

\[
\delta W_{j,\beta \alpha} \delta W_{j,\alpha \beta} \ll (\Lambda_{j,\beta} - \Lambda_{j,\alpha})^2
\]

(30)

As we note that an effect of \( D \) is \( W_{\alpha \beta} \rightarrow W_{\alpha \beta} D_{\alpha \alpha} D_{\beta \beta}^{-1} \) this criterion is independent of the choice of \( S \), \( D \) or \( \bar{D} \). Roughly, this means that when and if two eigenvalues of the transfer matrix are degenerate, any change in \( T \) that results in matrix elements / transitions between the nearly degenerate eigenvectors (in both directions) is particularly dangerous to the adiabatic approximation. This also suggests, however, that physical intuition depending on (in effect) Newton’s second law will be more robust if we arrange to choose \( D \) so that \( W_{\alpha \beta} \approx W_{\beta \alpha} \) and \( R_{\alpha \beta} \approx R_{\beta \alpha} \). Unfortunately, we have only \( n - 1 \) free parameters in \( D \), once we have insisted that \( \text{det} \left( S \right) = 1 \) and the above suggests \( n \left( n - 1 \right) / 2 \) equations on \( W \) and an equal number on \( R \). Moreover, any such criterion on \( R \), if we take \( \bar{D} = 1 \) will give local constraints on \( R \), but imply that, in order to calculate \( S \) we must take the product of all the \( R \)'s. For \( n = 2 \) this can be solved by insisting that \( W_{j,12} = W_{j,21} \) as the constraint on \( S_j \) or \( D_j \) and \( R_{j,21} = R_{j,12} \) as a constraint on \( \bar{D}_j \). Sensible criteria for larger matrices are likely to be that the largest / most important off-diagonal terms in \( W \) and \( R \) satisfy similar criteria. However, we do note that the final answers are in principle independent of \( D \), while \( \bar{D} \) only changes somewhat the order in time-dependent perturbation theory at which various terms contribute. Hence, details of these choices, given a sensible, local method for determining both \( S \) and \( R \) are probably essential only for very accurate work, and best choices will depend on the specific problem and specific objectives. In addition, these changes matter will matter only for changes to corrections to the leading order in perturbation theory. As, for our problems, we are primarily interested the leading order of perturbation theory to provide a first order approximation to problems that can accurately be modeled simply performing the matrix multiplications, we will not pursue this avenue further. More important to our work is the fact that the adiabatic approximation is likely to break down when two eigenvalues of the transfer matrix are degenerate. This possibility is discussed more below.
V. EXTENSIONS OF THE ADIABATIC APPROXIMATION

In the previous section we discussed the adiabatic approximations for products of large numbers of matrices and criteria for these approximations to be valid. In this section we discuss various ways in which this approximation can break down. In effect, these criteria are criteria on adjacent pairs of matrices. Clearly there are a number of possibilities. The simplest possibility to deal with is that a small number of pairs of matrices fail to satisfy the appropriate criteria, say $T_{k_i+1}, T_{k_i}$ for $K$ different values of $k_i$. In this case, we can simply use the formulae given above for the ranges in which the criteria are satisfied e.g. $k_1 \geq j \geq 0, \quad k_{i+1} \geq j \geq k_i, \quad N > j \geq k_K$, reducing the product of many matrices to the product of $K+1$ matrices. However, it is also possible that the criteria fail to be satisfied over a range of $j$ and/or that the range of $j$ over which these criteria fail to be satisfied is ill-defined: the criteria are satisfied increasing poorly over a range of $j$. This happens for a variety of reasonably common phenomena in physics: largely where the qualitative behavior of a problem changes as a function of the index $j$.

As a specific example we consider the Schrödinger-Verlet matrices

$$T^\text{Sch}_j = \begin{pmatrix} 1 & \Delta x_j \\ V_j \Delta x_j & 1 + V_j \Delta x_j^2 \end{pmatrix}. \quad (31)$$

If $\Delta x_j = \Delta x$ is a constant, then this matrix is the transfer matrix that corresponds to the Verlet approximation of the Schrödinger equation,

$$-\psi'' + V(x) \psi = 0, \quad (32)$$

provided that $V_j = V((j+1)\Delta x)$. If $\Delta x$ is not a constant, this is matrix still corresponds to a discrete approximation of this differential equation. However, rather than the error in the solution over the range $x_2 > \Delta x > x_1$ being $O(\Delta x^2 (x_2 - x_1))$ the error is rather $O(\Delta x^2 (x_2 - x_1), \Delta^2 x (x_2 - x_1))$ where $\Delta^2 x$ is a typical difference between the $\Delta x_j$. As this matrix has unit determinant, its eigenvalues satisfy $\Lambda_1 = \Lambda_2^{-1}$. It is easy to see that if $V$ is real, then in the “classically allowed” region, $V_j < 0$, these eigenvalues are complex conjugates on the unit circle, while in the classically allowed region $V_j > 0$ the eigenvalues are both real. Thus, there is an abrupt change in the qualitative behavior at $V_j = 0$, with many quantities, including the eigenvalues, eigenvectors and similarity transformations that diagonalize the matrix all having non-analytic $V^{1/2}$ behavior at the turning point. At the “classical turning
point” *V* 0 the matrix has two unit eigenvalues, can not be diagonalized, and has non-diagonal Jordan normal form. Moreover, it is easy to see that if we find a similarity matrix *S* a that diagonalizes *T* 11 for any classically allowed *V* < 0, however small *V*’s magnitude, and a similarity matrix *S* d that diagonalizes *T* 11 for any classically disallowed *V* > 0, however small *V*’s magnitude, then, *R* 11 = *S* 11 1 *S* -1 *c* can not be chosen to be close to unity and, in fact, if we insist on *det*(*R*) = 1, *R* 12 = *R* 21 and make the magnitudes of the relevant *V*’s arbitrarily small,

\[
R_t = \pm 2^{+1/2} \begin{pmatrix} 1 & -i \\ -i & 1 \end{pmatrix}.
\]  

Moreover it is easy to see that the criterion for the adiabatic approximation to be correct corresponds roughly to the region in which the semiclassical approximation or WKB approximation of the Schrödinger equation is valid. The WKB approximation for \( \psi \),

\[
\psi (x) = cV (x)^{-1/4} \exp \left( \int^x dx' V (x')^{1/2} \right) + c'V (x)^{-1/4} \exp \left( - \int^x dx' V (x')^{1/2} \right)
\]  

is valid provided \( V' \gg V^{3/2} \) e.g. not close to any turning point [7]. Similarly, the criterion for the adiabatic approximation for \( T^{11} \) fails when \( V \gg \Delta x V^{3/2} \). This provides convincing evidence that there is a rough correspondence between the adiabatic approximation for the product of matrices and the WKB approximation for a corresponding difference equation. More generally, for higher order differential equations (all non-trivial, relevant second order differential equations can be put in the Schrödinger form) the adiabatic criterion corresponds to the failure of a corresponding approximation on such differential equations, specifically on a result obtained by performing asymptotic balance on the Ricatti transformation of said equation. As it is well known that there are differential equations of this type that, despite intense interest for approximately a century, have not yet been satisfactorily solved, we immediately conclude that it will be impossible, in general, to deal with regions in which the adiabatic approximation fails. However, the situation in which there is a “simple” classical turning point \( x_t \) near which \( V (x) \approx a (x - x_t) \) is well approximated by the first term in its Taylor series, has been treated reasonably precise. This suggests that we ought to be able to deal with the situation in which a single pair of eigenvalues become equal, in a way qualitatively similar to that discussed above, by making an analogy to this prior work. In fact, we expect physically that this is the most usual “generic” way in which the adiabatic approximation can fail over a large region: two (and only two) eigenvalues approach each
other, with the trace of the relevant part of the matrix tending to zero linearly as a function of \(j\), with a corresponding square root singularity in the eigenvalues, eigenvectors etc.

To this end we note that it is well known that, in a region that contains a single turning point \(x_t\), \(V(x_t) = 0\) that the uniform asymptotic solution to eqn 32 is given by

\[
\psi_u (x; \{c, c'_0\}) = c_1 \psi_{u1} + c_2 \psi_{u2} = c_1 V^{-1/4} f^{1/6} A_i \left( \frac{3}{2} f \right)^{2/3} + c_2 V^{-1/4} f^{1/6} B_i \left( \frac{3}{2} f \right)^{2/3}
\]

where \(f = \int_{x_t}^x dx' V(x')^{1/2}\), \(A_i\) and \(B_i\) are the well known solutions to Airy’s equation (eqn 32 with \(V = x\)) and the branch cuts of the various fractional powers can (and must) be taken in such a way that this function is analytic [8]. In particular

\[
\frac{-\psi''_u + V \psi_u}{(V \psi_u)} = -\frac{5}{36 f^2} + \frac{5 V''}{16 V^3} - \frac{V'''}{4 V^2}.
\]

Far from the turning point this ratio it is simply that \(f \gg 1\) augmented by the (second order) criterion for validity of the WBK approximation. In a small region near the turning point this ratio diverges, proportional to \(V\) (although this is not obvious). However, the characteristic length scale over which \(\psi\) is is expected to change is \(V^{1/3}\) and, for small \(y = (x - x_t) V^{-1/3}\)

\[
\frac{-\psi''_u + V \psi_u}{(V \psi_u)} \approx -\frac{72 V'' + 45 V''' V'''}{70 y V^{7/3}}
\]

Provided that this ratio is small when \(y\) is still small, the errors in the solution will also be small, resulting limits of order unity on the second and third derivatives of \(V\), when scaled by \(V\).

We write the solution to the difference equation 15 in for the Airy transfer matrix (eqn 31) to good approximation as linear combinations of Airy functions with arguments consistent with the uniform asymptotic expansion eqn 35. In doing this we may (for accuracy) remember that the Verlet approximation assumes that the derivative is given at points half way between the points at which the function is given. Then, if we write

\[
\phi_j = \begin{pmatrix} \psi_u(x_j) \\ \psi'_u(x_j + \frac{1}{2} \Delta x_j) \end{pmatrix}
\]

with an appropriate choices for \(f\) we expect that the values of \(c_j\) and \(c'_j\) will be essentially constant for all \(j\). From the point of view of the transfer matrix, this means that if we make a \(j\) dependent linear transformation to a basis in which we have solved eqn 38 for the
components of $\phi_j$ in terms of $c_j$ and $c'_j$ then we expect that the transfer matrix, in this new basis, will be essentially unity. Note that in the region where the adiabatic approximation is valid and the eigenvalues of the transfer matrix are real, we expect that the this “Airy” basis corresponds to the basis in which the transfer matrices are diagonal; where the eigenvalues are complex conjugates, these bases correspond only when we solve for $c \pm ic'$. Thus, if we make the transformation,

$$
S^A_j = \begin{pmatrix} 
\psi_{u1} (x_j) & \psi_{u2} (x_j) \\
\psi'_{u1} (x_j + \frac{1}{2}\Delta x_j) & \psi'_{u2} (x_j + \frac{1}{2}\Delta x_j)
\end{pmatrix}^{-1}
$$

we expect the transformed transfer matrix to be effectively unity everywhere, even in the turning point region. If we can, further, find a correspondence between the Airy transfer matrix and a general transfer matrix, this will allow us to transform these transfer matrices to a basis in which they are effectively unity even in the turning point region.

First we consider how to relate the general transfer matrices for the product of which we want to calculate to the Schrödinger-Verlet transfer matrix of eqn 31. We consider first the possibility that $n = 2$ and that there is exactly one turning point. We then make a correspondence between a general $2 \times 2$ transfer matrix $T_j$ and the Schrödinger-Verlet transfer, and calculate the appropriate values of $V_j, \Delta x_j$ and $f_j$ and, finally, give a formula which, in principle allows determination of the errors in use of these formulae. First we note that the determinant of the Schrödinger-Verlet matrix is unity. As the eigenvalues of the equation is essential to the adiabatic approximation far from the turning point it seems essential to preserve the eigenvalues. However, this can be done simply by multiplying the Schrödinger-Verlet matrix by the determinant of the general matrix and insisting that the ratio of the eigenvalues of the general and Schrödinger-Verlet matrices are equal. The product of the determinants of the original transfer matrices are, of course, simply constants and so simply multiply the final answer. The ratio of the eigenvalues of the Schrödinger-Verlet matrix is a function only of its trace, $2 + V_j \Delta x_j^2$ which can then be determined from

$$
2 + V_j \Delta x_j^2 = Tr (T_j) / det (T_j)^{1/2}
$$

In doing this we have assumed that we have chosen the square root of $det (T_j)$ so that $Re \left[ Tr (T_j) / det (T_j)^{1/2} \right] > 0$. If both the eigenvalues of the original matrix $T_j$ have negative real part, this results in significantly different behavior for the difference equation, although
the results quoted below are still accurate. Moreover, there are cases, for example the middle of the band-gap in a dielectric mirror, when continuity results in a change in sign in the real parts of the eigenvalues of the original matrix. In this needs to be taken into account in apply the formulae below. In the context of eqns 25 and 17 it is clear that if we consider two sequential $2 \times 2$ matrices $T_j, T_{j+1}$ there are, in addition to the determinants of the matrices and their traces, or, equivalently, ratio of eigenvalues, one more basis independent quantity, $W_{12}/W_{21}$. This can be determined from $\frac{\text{Tr} (T_{j+1} T_j)}{\sqrt{\det (T_{j+1}) \det (T_j)}}$ yielding the result
\[ V_{j+1} = \frac{1}{2} \left( \tau^2 - \tau \sqrt{\tau^2 - 4} - 2 \right) V_j \] where
\[ \tau = \frac{\text{Tr} (T_{j+1} T_j) - \frac{1}{2} \left( \text{Tr} (T_{j+1}) \text{Tr} (T_j) - \left( \text{Tr} (T_{j+1}) - 2 \sqrt{\det (T_{j+1})} \right) \left( \text{Tr} (T_j) - 2 \sqrt{\det (T_j)} \right) \right)}{\sqrt{\det (T_{j+1}) \det (T_j)} \sqrt{\left( \text{Tr} (T_{j+1}) - 2 \sqrt{\det (T_{j+1})} \right) \left( \text{Tr} (T_j) - 2 \sqrt{\det (T_j)} \right)}} \] (42)

This still does not allow us to determine the initial value of $V_j$ in a string of Schrödinger-Verlet matrices. However, this simply reflects a re-scaling of the Schrödinger equation, also reflected by a similarity transformation of the Schrödinger-Verlet matrices along with taking $V \rightarrow V \lambda^{-2}, x \rightarrow x \lambda, \Delta x \rightarrow \Delta x \lambda$. These formulae then allow us to relate an arbitrary set of $n = 2$ transfer matrices to a specific set of Schrödinger-Verlet matrices. Note that these choices imply that $\Delta x_j$ is a function of $j$ and in consequence that “Verlet” is a misnomer-- a true Verlet approximation will have errors of order $\Delta x^2 (x_f - x_i)$ where $\Delta x$ is the step in $x$, $x_f$ is the final value for $x$ and $x_i$ is the initial value thereof. However, if $\Delta x$ varies, this is really only a procedure that has errors of order $\Delta x^2 (x_f - x_i)$ where $\Delta x$ is a typical value of the step in $x$ and $\Delta x^2$ is a typical measure of the variation therein. This accuracy can probably be improved by re-interpretation of this matrix in terms of a more complicated numerical procedure. However, it is adequate for our purposes so this complication is suppressed.

The implied products of these matrices are intended to be the same, up to a similarity transformation. In fact, however, we need still to notice that, while any two successive matrices are determined, up to a similarity transformation by one parameter in addition to their eigenvalues, this pair of matrices together with the constraint that the similarity transformation have unit determinant completely determines this similarity transformation.
We then need an additional freedom, as reflected e.g. by \( D \), for a sequence of matrices as in eqn 18. While a precise examination of the problem would require a determination of \( D \), it is important to note that this function depends on three successive transfer matrices. Thus, in effect it is a second difference of the transfer matrices. Thus this term is reasonably considered a higher order effect than those considered in this paper.

Having made this relationship the remaining task in determining our product is to determine remaining unknown parameters in \( S^{Ai} \). These include the exact discretized versions of \( \psi_{ja} \) and \( \psi_{ja}^- \). It seems clear that we should approximate \( f \) as the discrete sum related to the given integral, but still need a location for the turning point. Other than this, the detailed value for \( S^{Ai} \) is unimportant except in the turning point region, as it must be chosen to have appropriate limits where the adiabatic approximation is appropriate. Products that end at a turning point. It is easy to find the location of the turning point to within two values of the index \( j \): in the physically usual case that the ratio of the eigenvalues goes from a real number to a number on the unit circle, there will be two consecutive values of \( j, j_i \) and \( j_i+1 \) for which this happens. For other situations for which the eigenvalues are always complex, there are two consecutive values of \( j \) between which there is a square root singularity in the eigenvalues / for which \( Tr (T_j) / det (T_j) \) passes through 2. We will deal with these two matrices separately. For the remainder of the region of interest we intend to use

\[
\prod_j T_j^{Ai} = \prod_j \left( S_j^{Ai} \right)^{-1} S_j^{Ai} T_j^{Sch} = \prod_j R_j^{Ai}
\]

where \( T_j^{Sch} \) is the Schrödinger-Verlet transfer matrix corresponding to \( T_j \), and we are intent on arranging that \( R_j^{Ai} = S_j^{Ai} T_j^{Sch} \left( S_j^{Ai} \right)^{-1} \) is close to unity. To determine \( S_j^{Ai} \) we still need to determine the details of its matrix elements. We suggest:

\[
\psi_{ja} = V_j^{-1/4} f_{j+1/2}^{1/6} Ai_2 \left( \left( \frac{3}{2} f_j \right)^{2/3} \right)
\]

and

\[
\psi'_{ja} = \left( \frac{3}{2} \right)^{-\frac{7}{6}} \left( V_j^{1/2} f_j^{-\frac{1}{2}} \right) V_j^{-1/4} f_{j+1/2}^{1/6} Ai_2' \left( \left( \frac{3}{2} f_j^{1/2} \right)^{2/3} \right)
\]

where \( Ai_1 \) is the Airy \( Ai \) function and \( Ai_2 \) is the Airy \( Bi \) function (or, alternatively, an appropriate linear combination) \( f_{j+1} = f_j + \Delta f_j, f_{j+1/2} = f_j + \frac{1}{2} \Delta f_j \) and \( \Delta f_j = \Delta x_j V_j^{1/2} \), which can be calculated exclusively from the eigenvalues of \( T_j \). These formulae need some explanation. The difference equations for \( f_j \) are natural: \( f_j \), like \( S_j^{Ai} \), can be thought
of as being centered between the matrices $T_j, T_{j+1}$, while $\Delta f_j$ is centered on $T_j$, making these (mostly) centered difference equations. Consistent with the Verlet approximation, we have centered $\psi$ on the “points” and $\psi'$ on “half points”, except for the prefactors $V_j \frac{1}{2} f_j \frac{1}{2}$, which, actually, are expected to change slowly so that including their differences between points and half points seems irrelevant. Finally, \((\frac{3}{2})^2 \left(V_j f_j \frac{1}{2}\right)\), the derivative of \((\frac{3}{2} f_j + \frac{1}{2})\) is conveniently (and appropriately) evaluated at half points. Moreover this choice, together with the fact that the Wronskian $W[\psi(x), \psi'(x)] = \pi^{-1}$ implies that

$$
\text{det} \left(S_j^{\psi}\right) = \pi^{-1} + O\left(\Delta f^2\right)
$$

\hspace{1cm} (46)

with the error coming from the fact that the Airy function and Airy function derivatives are evaluated at different arguments and that the first correction term in this difference has determinant zero. With these assumptions, it is not difficult to show that $R_j^{\psi}$, is close to unity, assuming that $\Delta x_j$ is small and that neither $V_j$ nor $\Delta x_j$ changes too rapidly with $j$.

The detailed calculation of this fact is relatively simple when preformed by Mathematica or a similar automated algebra routine is not difficult and we find that the errors are, as suggested above, $O\left(\Delta f^3, \Delta f^2 \left(\Delta x_j - \Delta x_{j+1}\right)\right)$. The specific formulae are quite complicated. Also, it is not expected that it would be a routine matter to use such formulae: the product of the $R^\psi$'s is too complicated to calculate to make taking this product to calculate small changes to the final answer a routine matter. It is of some interest to know the approximate prefactors of the given orders for the errors, but these are more often suppressed in initial treatments. Moreover, we believe that there are better choices for $S^\psi$, that give more precise results, specifically that accommodate a true second order solution of the Schrödinger equation or (possibly equivalently) allow for an additional freedom in the similarity transformation $S^\psi$.

For all these reasons, the detailed formula is not given here.

It remains to calculate $f_{j+1}$ and $f_{j-1}$, which, in some sense is the primary objective of the discussion here: it will be our main result that will survive in final answers of interest. There are, in principle three cases of interest. First: $f_{j+1}$ and $f_{j-1}$ are both small, second, one is small and the other is of order unity, lastly both are of order unity. If both are of order unity, then the adiabatic approximation is valid everywhere except at the point between $T_j$ and $T_{j+1}$. In this case we need simply use the adiabatic approximation everywhere except to include a value for $R_j$, which (generally) we would expect to be not close to unity but rather to be similar to 33. The possibility that one of these is small and the other is not is the
most unusual circumstance and will not be addressed here. Roughly this likely implies that the adiabatic approximation is valid everywhere except exactly at the turning point or that there is a sudden change in the rate of change in the transfer matrices $T_j$. If, on the other hand both are small, then we can determine $T_{j+1}^{Sch}$, $T_{j+1}^{Sch}$ then looking for a transformation that makes $\Delta f_{j+2}$ in order to determine

$$S_{j+1}^{Ai} T_{j+1}^{Sch} T_{j}^{Sch} \left(S_{j-1}^{Ai}\right)^{-1}.$$  \hspace{1cm} (47)

This is a term that should be included in the product that we are calculating; in effect it is the product of the two $R^{Ai}$ nearest the turning point. Moreover, we expect that the turning point should (notionally) be in the region where these transfer matrices approximate the underlying Schrödinger equation. A precise location for the turning point, therefore, can be determined by making this product as close to unity as possible, consistent with ease of computation. The simplest possibly is simply to “declare” the turning point to be at the point between the two transfer matrices: another possibility would to take the turning point to be notional at the point at which the potential is zero, assuming a linear interpolation of thereof between the points at which it is “known” to the Schrödinger-Verlet equation, e.g.

$$x_t = x_{j_t} + \frac{1}{2} \Delta x_{j_t} + 2V_{j_t} \left(V_{j_t+1} - V_{j_t}\right)^{-1} \left(\Delta x_{j_t+1} + \Delta x_{j_t}\right)$$ \hspace{1cm} (48)

$$x = x_{j_t} + \frac{1}{2} \Delta x_{j_t} + 2V_{j_t} \left(V_{j_t+1} - V_{j_t}\right)^{-1} \left(\Delta x_{j_t+1} + \Delta x_{j_t}\right).$$

The final and most accurate possibility is to expand the product of 47to low order in $f_{j+1}$ and $f_{j-1}$, and other variables such as $V_{j_t+1}$ on which this product depends, and adjust these variables so that the product is close to unity. Details of this more accurate final calculation, including the exact sense in which this product should be close to unity, have not been completed at this time. However, all of the above, including (simply) using the Airy functions with a centered turning point are, to the best of our knowledge advances on the present literature for dielectric mirrors and Rydberg atoms. These have left out even the $O(\Delta x^0)$ contributions to the results coming from the shift in the apparent location of the turning point coming from the $\pi/4$ terms that appear in the asymptotic expansions of the Airy functions for large arguments. The centered approach discussed above will account for this correction exactly, the interpolation approach of eqn 48 should get results including corrections of order $\Delta x$. Appropriate treatment of eqn 47 should not merely have the advantage of including terms up to order $\Delta x^2$ but will also be relatively insensitive to large step sizes near the turning point: in effect making this term close to unity is, finally, what determines the error near the turning point.
VI. CONCLUSIONS

In this paper we have examined the behavior of the product of a large number of slowly varying matrices, in the particular context of random and non-random dielectric mirrors. At the lowest level of an adiabatic approximation we find that it is possible to relate this product of matrices to the similarity transformations that diagonalize the first and last matrix, together with the eigenvalues of the matrices between them. This is a great advance as it is commonly quite easy to calculate or at least approximate these eigenvalues analytically. This, in turn will allow use of such formulae in the design of complicated chirped mirrors in which many parameters such as the index contrast between layers, the thickness of each successive layer and one or more measures of randomness to be including in simple formulae addressing the engineering design of such mirrors.

While a specific analysis mapping out the regions of interest for such random chirped adiabatic dielectric mirrors was our intention when we started this work, we discovered while approaching it that we could not find an aspect that we wanted to treat in the literature: this aspect was a “turning point” and near which two eigenvalues of the matrix are equal or close to each other. Such points, which for mirrors correspond to band edges, result in a break-down of the adiabatic approximation. Looking at this behavior in the light of a discrete version of the Schrödinger equation it became apparent that any approximation that treated points of this nature well would require a treatment at least as complicated as the Airy “matching formulae” from the semi-classical treatment of the Schrödinger equation. Such a semi-classical treatment for the Schrödinger corresponds to the simple adiabatic approximation when this is valid but gives also gives a good approximation to the matrix product in the turning point regime. This, in turn, will allow treatments of matrix products with such turning points, which seem not to have been given in the past. This will again allow simple operations on eigenvalues able to be found analytically, and on a single additional parameter, given for $2 \times 2$ matrices near a simple turning point by eqn 41, and finally by a parameter that gives the location of the turning point, to determine more precisely the properties of chirped dielectric mirrors somewhat more generally. In comparison to the treatments of chirped dielectric mirrors that are available in the literature, which typically start from a WKB like treatment of a continuum theory [9], these results should be appreciably more accurate for such properties as the phase delay as a function of frequency in
chirped mirrors. Unfortunately time constraints implied that we could did not complete a determination of a best method for determining the location of the turning point. Moreover, the turning point methods will need extension in chirped, random dielectric mirrors for which the eigenvalue structure is potentially appreciably different. Both these issues will be a matter for future work, as will the detailed treatment of the initial problem we intended to address: the simple chirped mirror, using the discrete transfer matrix method rather than continuous ones.