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Quasiclassical Wavefunctions

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A convergent quasiclassical formula for the wavefunctions of a closed quantum or wave system is obtained. This is expressed entirely in terms of classical orbits. The result is at the same level as earlier results expressing the spectrum as a finite resurgent sum over composite periodic orbits.

KEY WORDS: Quasiclassical; semiclassical; wavefunctions; periodic orbits; Fredholm theory; surface of section.

I. INTRODUCTION

The quasiclassical approximation [QCA] in quantum or wave systems exploits the smallness of the parameter λ/a, where λ is the wavelength and a is a typical classical length. The classical limit of vanishing wavelength is very singular, however. For example, the classical limit does not commute with other interesting limits, in particular the long time limit, used to define chaos or sharp energy levels. As a result, the formal series for quantum amplitudes are often not absolutely convergent and thus can take on any value desired, depending on the order of summation. This difficulty is particularly acute when the classical limit is chaotic. These difficulties are present in the well known Gutzwiller trace formula,[1] which expresses the density of states as a sum over WKB amplitudes, similar to Eq. (2) below. The difficulties have been overcome in cases where the prefactors are simple enough, especially for the case of strong hyperbolic chaos, where all orbits are hyperbolically unstable.[2–6]

For the spectrum, the orbits of interest are the periodic orbits. Of course, only the canonically invariant properties of the orbits, i.e., the actions and the stabilities, can affect the spectrum. The basic technique was a "resummation" of Gutzwiller's series into a dynamical or Gutzwiller–

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Voros zeta function, or "spectral determinant," which vanishes on the spectrum. The zeta function was expressed as an infinite product, reminiscent of Riemann's zeta function. This product also does not converge, but a variety of arguments have been put forward giving prescriptions for a correct expansion, corresponding to the Dirichlet series in the theory of the Riemann zeta function. Thus, the spectral problem for hard chaos, in the QCA context, has been solved, or at any rate the most glaring mathematical difficulties are avoided. A rigorous account is not at hand, however.

Recently, we put forward a general technique, based on Fredholm integral equations, applicable to this problem, but also to problems of mixed chaos and integrable systems as well as to scattering.[7-9] The technique can give convergent expressions for matrix elements and wavefunctions, as well. In this article we produce a convergent formula for the wavefunctions of closed systems which is expressed entirely in terms of classical orbits.

II. THE ENERGY GREEN'S FUNCTION

We study the Green's function at constant energy, from which we can extract the wavefunctions. This is expressed in terms of wavefunctions and energies, [for a closed system], by

$$G(\mathbf{r}_1, \mathbf{r}_2, E) = \sum_a \frac{\Psi_a(\mathbf{r}_1)\, \Psi_a^*(\mathbf{r}_2)}{E - E_a + i\eta} \tag{1}$$

The Van Vleck expression[10]

$$G(\mathbf{r}_1, \mathbf{r}_2, E) = \sum_{paths} \frac{1}{ih} \left[\frac{1}{2\pi i h v_1 v_2} \left| \frac{\partial^2 S_p}{\partial r_{1\perp}\, \partial r_{2\perp}} \right| \right]^{1/2} \exp\left[\frac{i}{h} S_p(\mathbf{r}_1, \mathbf{r}_2, E) - i \frac{\pi}{2} \nu_p \right] \tag{2}$$

for the same Green's function in the QCA is based on classical orbits, as desired, but is mathematically and even physically somewhat dubious. It is the Feynman path integral expression for the same object, evaluated in the stationary phase approximation. If Eq. (2) is correct, then, for almost all points $\mathbf{r}_1, \mathbf{r}_2$, the series must diverge as $E \to E_a$, i.e., the long orbits must dominate the sum, and these must contrive to diverge at the same energies independent of end points. While it is reasonable that precise energy levels are related to long time behavior, it is known empirically that most of the contribution comes from short orbits. In any case, the number of very long orbits (taking time $T_p = \partial S_p / \partial E$) are exponentially numerous, in the chaotic case, going as $\#(T_p) \approx \exp(\gamma T_p)/T_p$, so there are an enormous

number of orbits whose actions S_p lie between a given S and $S+\hbar$. There is no particular point in distinguishing between these orbits. We shall see that this can be exploited to express long orbits as compositions of shorter ones, allowing the theory to be expressed entirely in terms of a finite number of classical orbits.

Our theory is based on the following exact integral expression for the Green's function:

$$G(\mathbf{r}, \mathbf{r}', E) = G_0(\mathbf{r}, \mathbf{r}', E) + \int_{SS} dq\, V_-(q, \mathbf{r}, E)\, \mu(q, \mathbf{r}', E) \tag{3}$$

The quantity μ obeys a *Fredholm integral equation*[11]

$$\mu(q, \mathbf{r}', E) = V_+(q, \mathbf{r}', E) + \lambda \int_{SS} dq'\, K(q, q', E)\, \mu(q', \mathbf{r}', E) \tag{4}$$

The integral is over a $d-1$ dimensional subspace, a *surface of section*, *SS*. A typical example is shown in Fig. 1a. The quantities μ, $V_\pm$ depend parametrically on $\mathbf{r}$, E, the kernel K depends on E, and G_0 is the free space Green's function. The bookkeeping parameter λ eventually is set equal to unity. Figure 1u, d suggests one important technique for obtaining such exact kernels. Integral equations of this type have been derived in the present context in refs. 4, 6, and 12.

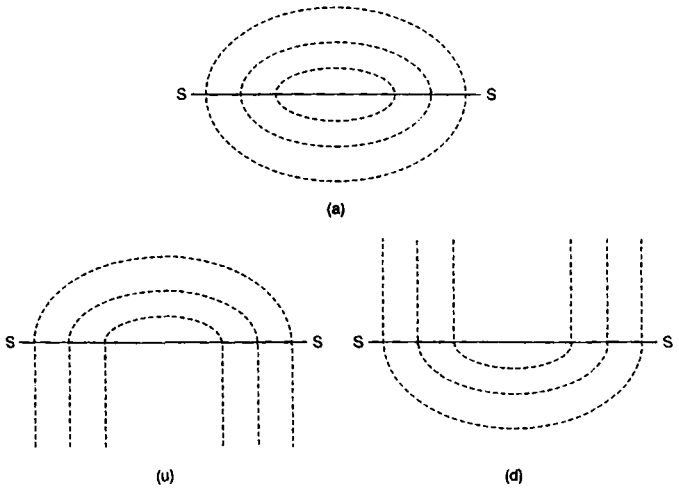

Fig. 1. (a) Schematic of a surface of section, S-S, in an elliptic potential well. (u), (d) Auxiliary scattering potentials. The Green's functions and/or scattering operators of these auxiliary potentials can be combined to give an exact kernel for the surface of section shown in (a).

There are several virtues to this formulation. First, equations of this form are mathematically and numerically well studied, and most difficulties have been overcome. Second, the integrals are over a one-dimensional subspace, [or more generally for a d-dimensional problem, a $d-1$ dimensional subspace]. This is effectively a wave generalization of the classical Poincaré surface of section. It is also a generalization of the boundary integral method which is in widespread use for billiard problems.[13] Numerical discretization of these equations needs a one dimensional rather than a two dimensional grid or element representation. Third, there are many, indeed infinitely many, exact equations of this form which solve the same problem. There are many choices of surface of section, and many representations of the kernel. True, most of these give rise to intolerably complex and sensitive kernels and auxiliary functions, but it does allow much scope for ingenuity and it gives a way to exploit special features of the problem at hand. [For brevity, in the following we sometimes use the term "kernels" to refer not only to K but to G_0 and the V's as well.] Also, to find the kernels it is usually necessary to solve an integral equation as difficult as the original problem. However, the QCA approximation to the kernels can be quite simple and accurate, since the kernels represent the contribution of short orbits, e.g., orbits having just one encounter with the surface of section. We shall assume that there is just one orbit contributing to the kernel, for brevity of notation. We shall also keep just the leading order approximation, although this is also a good method to study corrections to the leading order.

A formal expression for the solution of (4) is

$$\boldsymbol{\mu} = \frac{\mathbf{1}}{\mathbf{1} - \lambda \mathbf{K}} \mathbf{V}_+ \tag{5}$$

so that the crucial construct is the inversion of the operator $\mathbf{1} - \lambda \mathbf{K}$. The simplest way to invert this is by the *Neumann series*, valid if $\|\lambda \mathbf{K}\| < 1$, that is,

$$\frac{\mathbf{1}}{\mathbf{1} - \lambda \mathbf{K}} = 1 + \lambda \mathbf{K} + \lambda^2 \mathbf{K}^2 + \cdots = \sum_{n=0}^{\infty} \lambda^n \mathbf{K}^n \tag{6}$$

The Gutzwiller trace formula, and the more general Van Vleck Green's function formula are approximations at the level of the Neumann series. The Van Vleck formula (2) is recovered by a) making the QCA approximation for the kernels, which are then expressed in the *prefactor* $\times$ $\exp(iS/\hbar)$ form, [or as a sum over such terms]. This is followed by doing all the integrals in Eqs. (3), (5), and (6) by the method of stationary phase. We shall assume that it has been possible to choose the surface of section

and kernel sufficiently astutely that only real orbits are needed. Then the Van Vleck series is organized into groups of orbits according to how many time the orbit crosses the surface of section, incidentally providing a definite mathematical prescription for the series, which so organized either diverges or converges. In fact, the Neumann series often does not converge. Indeed, when $E = E_a$, $\mathbf{K}$ has a unit eigenvalue, and the series diverges at the physical value of $\lambda = 1$.

The exact solution obtained by Fredholm almost a hundred years ago is physically quite formal, although it is mathematically explicit and well behaved, being expressed in terms of a *ratio* of *absolutely convergent* power series in λ whose coefficients are expressed as integrals of certain determinants. Thus,

$$\frac{\mathbf{1}}{\mathbf{1}-\lambda\mathbf{K}} = \frac{\mathbf{N}(\lambda)}{D(\lambda)} = \frac{\sum_{n=0}^{\infty} \lambda^n \mathbf{N}_n}{\sum_{n=0}^{\infty} \lambda^n D_n} \tag{7}$$

A better way of computing these coefficients is through the recurrence relations

$$D_n = -\frac{1}{n} \sum_{r=1}^{n} \sigma_r D_{n-r} \tag{8}$$

and

$$\mathbf{N}_n = \sum_{r=0}^{n} \mathbf{K}^r D_{n-r} \tag{9}$$

where

$$\sigma_r = \operatorname{Tr} \mathbf{K}^r \tag{10}$$

Equation (8) is effectively the relation $\ln \det(\mathbf{1} - \lambda\mathbf{K}) = \operatorname{Tr} \ln(\mathbf{1} - \lambda\mathbf{K})$.

Thus

$$G(\mathbf{r}, \mathbf{r}') = G_0(\mathbf{r}, \mathbf{r}') + \iint dq\, dq'\, V_-(\mathbf{r}, q) \frac{N(q, q')}{D(E)} V_+(q', \mathbf{r}') \tag{11}$$

In general, G_0 accounts for orbits which do not cross the surface of section, V_+ accounts for orbits leaving $\mathbf{r}'$ and arriving for the first time at the SS at point q' and V_- takes care of the orbits which leave the SS at point q, arriving at $\mathbf{r}$ without crossing the SS in between. As a rule, the shorter the SS, the more complicated these objects become.

III. QUASICLASSICAL APPROXIMATION

To this point, the formulation is exact. We now turn to the quasiclassical approximation. The first step is to replace the exact kernel **K** by its quasiclassical or asymptotic approximation, which we call **T**. The general form of **T** is

$$T(q, q', E) = \sum_b \frac{1}{\sqrt{2\pi i\hbar}} \sqrt{\left| \frac{\partial^2 S_b(q, q')}{\partial q\, \partial q'} \right|}\, e^{(i/\hbar) S_b(q, q')} \tag{12}$$

The sum is over classical orbits b of energy E, action S_b, going from one point q' on the surface of section to another point q, without crossing the surface of section in between. [We incorporate the Maslov phase into the definition of the action, S_b.] We will also replace G_0, $V_\pm$ by their quasiclassical approximations, which have a similar form, although we won't give them new names.

The connection with classical mechanics comes because $S_b(q, q')$ is the generator of the *classical surface of section map* $(q, p) = \mathscr{T}(q'p')$ carrying an initial point q', with momentum p' parallel to the section, to a final point q, p. The map $\mathscr{T}$ is found by solving the equations $p = \partial S_b(q, q')/\partial q$, $p' = -\partial S_b(q, q')/\partial q'$.

The D_n's are represented in terms of the traces

$$\sigma_n \approx \tau_n = \operatorname{Tr} \mathbf{T}^n = \int \cdots \int dq_1 \cdots dq_n T(q_1, q_2) \cdots T(q_n, q_1) \tag{13}$$

Carrying out the integrals in stationary phase approximation gives expressions for τ_n which are expressed as a sum over periodic orbits of "SS length" n. A particular orbit can be primitive or it can be an r-fold repetition of some shorter orbit of SS length s with $n = rs$. If the orbit is *isolated*, all the integrals will have rapidly varying phases. For such orbits

$$\tau_n = \sum_{r, s;\, rs = n} s\, |\det[(M_s)^r - 1]|^{-1/2} \exp \frac{i}{\hbar} r S_s(E) \tag{14}$$

Here S_s is the action and M_s is the monodromy or stability matrix for the primitive orbit. For an unstable orbit M_s has eigenvalues Λ_s, Λ_s^{-1} with $|\Lambda_s| > 1$. Most work on periodic orbit theory confines itself to this case of hard chaos. If all traces can be so expressed, the Gutzwiller series is given by the expansion of the logarithmic derivative $\partial \ln D(E)/\partial E$, where, in the spirit of stationary phase, the derivative is regarded as acting only on $S_p(E)$.

Thus, in the nth coefficient D_n are grouped all combinations of periodic orbits whose SS length totals to n. Such combinations are called *composite* orbits, or less descriptively, pseudo orbits. A periodic orbit which does not repeat itself, is called a *prime* or primitive periodic orbit, and composite orbits are composed of prime orbits. This corresponds to the notion of prime and composite numbers. In fact, in the theory of the Riemann zeta function, S is $\ln n = \ln \prod p^{m_p} = \sum m_p \ln p$, and the Dirichlet series for Riemann zeta function corresponds to the orbit approximation of a Fredholm determinant.

Using the QCA approximations for $V_\pm$ we may express Eq. (11) in terms of a new type of composite orbit. The denominator was just discussed. The new type of orbit is in the numerator. It consists of a single *propagating orbit*, composed with one or more *periodic* orbits. The total SS length of the composite orbit is just the total number of SS crossings of all orbits in the composite. The composite orbits of the same length are grouped together in the terms of the final formulas, Eqs. (40) and (41), below.

IV. FINITENESS OF THE QCA

The T operator given above in Eq. (12) has an interpretation in terms of classical orbits. Within the framework of the QCA it has another property of importance: Namely, it is of *finite rank*.

The representation of the kernel T is arbitrary so we may write

$$T(q, q') = \sum_{mn} \phi_n^*(q)\, T_{nm} \phi_m(q') \tag{15}$$

where the ϕ's are a complete orthonormal set of states on the surface of section. The kernel is of finite rank N, if there exists a representation of the form Eq. (15) such that only N terms in each sum are nonvanishing, and N is the smallest number for which this is true. Kernels of finite rank are equivalent to finite matrices, although in arbitrary representations they have an arbitrarily large number of nonvanishing matrix elements.

If the surface of section is a simple closed curve, then a natural basis set is the Fourier basis, $\phi_n(q) = L^{-1/2} e^{2\pi i n q/L}$, where L is the length of the SS. Now,

$$T_{nm} = \frac{1}{L} \iint dq\, dq'\, e^{2\pi i (mq' - nq)/L} T(q, q') \tag{16}$$

an integral that can be estimated in SΦ. The stationary points are found by solution of the equations $2\pi n\hbar/L = \partial S(q, q')/\partial q = p$, $2\pi \hbar m/L = -\partial S(q, q')/\partial q' = p'$. For given energy, the classical momenta p, p' typically have a maximum

momentum magnitude $|p_o|$. This implies that stationary points exist for $|n| \leqslant |p_o|\, L/h = L/\lambda$, where λ is the magnitude of the shortest wavelength at energy E. If there is no stationary point, the integral is quasiclassically small. Therefore, the matrix elements T_{mn} in this representation are only large in an $N \times N$ submatrix where $N = 2L/\lambda$. Similar results are expected to hold with more general surfaces of section.

The consequences are straightforward. First, the coefficients D_n *vanish quasiclassically* for $n > N$, and the coefficients N_n vanish for $n \geqslant N$. In other words, the composite periodic orbits of SS length n, added up according to the rules for calculating D_n, systematically cancel leaving a quasiclassically small residue, for $n > N$. The typical composite orbit of SS length N has a real composite period of order the Heisenberg time. This was shown explicitly for the case of hard chaos by Bogomolny.[4] It agrees with the result of Berry and Keating[5] who find that contributions of composite orbits of period greater than the Heisenberg time are quasiclassically small.

Perhaps more surprisingly, we may express the Green's function $G(\mathbf{r}, \mathbf{r}', E)$ by means of Eq. (11) quasiclassically in terms of orbits of energy E from point $\mathbf{r}'$ to point $\mathbf{r}$. Composite *propagating* orbits combining such *nonperiodic orbits* with *periodic orbits* may be accordingly defined and grouped according to their SS-length. Such combinations of composite propagating orbits *vanish quasiclassically* for $n \geqslant N$.

The physics of this was well known for some time, but no one had found a way to exploit it before the introduction of the Fredholm method.[7] Namely, long propagating orbits, i.e., those crossing the SS many times, must necessarily be close to periodic orbits over much of their trajectory. Therefore, long propagating orbits can be well approximated by shorter propagating orbits with the same endpoints which are composed with periodic orbits. Thus to leading quasiclassical order, all Green's functions, and scattering amplitudes, can be expressed as a sum over a *finite number of orbits.*

V. UNITARITY OF THE *T* OPERATOR

In the preceding section we found that, up to quasiclassical errors, T_{mn} is a finite matrix. We next argue in the case of a *closed system*, T_{mn}, [restricted to the subspace where T does not vanish] is *unitary*, again up to quasiclassical errors. Indeed, using Eq. (12) we find that

$$\int dq\, \bar{T}(q, q_1)\, T(q, q_2) = \frac{1}{2\pi\hbar} \int dq \left[\frac{\partial^2 S}{\partial q\, \partial q_1} \frac{\partial^2 S}{\partial q\, \partial q_2} \right]^{1/2} e^{(i/\hbar)(S(q, q_2) - S(q, q_1))} \quad (17)$$

where the bar indicates complex conjugation. The phase will be stationary only for $\partial S(q, q_1)/\partial q = \partial S(q, q_2)/\partial q$, i.e., only if the classical orbits from q_i to q have the same final momentum. Since the orbits are unique, the phase is stationary only for $q_1 = q_2$. Expanding, $S(q, q_2) \cong S(q, q_1) + (q_2 - q_1)\, \partial S(q, q_1)/\partial q_1$, we find

$$\int dq\, \bar{T}(q, q_1)\, T(q, q_2) = \frac{1}{2\pi\hbar} \int dp\, e^{(i/\hbar)\, p(q_2 - q_1)} \cong \delta(q_1 - q_2) \tag{18}$$

where $p(q) = \partial S(q, q_1)/\partial q_1$. The integral is not strictly a δ-function because the effective limits are $\pm |p_o|$, but it can be treated as one within the QCA.

Thus, making only quasiclassical errors, we can treat Bogomolny's **T** operator as a *unitary* operator of *finite rank N*. The same result is obtained by Doron and Smilansky who formulate the problem in terms of scattering matrices, which also are of finite rank. This unitarity corresponds to the *functional relation* for $Z(E)$ used by Berry and Keating.

VI. RESURGENCE IN THE SPECTRAL DETERMINANT

The consequences of this unitarity are fairly straightforward. Using $D(\lambda) = \det(1 - \lambda \mathbf{T})$, where **T** is an $N \times N$ unitary matrix, and λ is real, we have

$$\bar{D}(\lambda) = \det(\mathbf{1} - \lambda \mathbf{T}^{-1}) = \lambda^N \det(-\mathbf{T}^{-1}) \det(\mathbf{1} - \lambda^{-1}\mathbf{T}) = e^{-i\Phi} \lambda^N D(\lambda^{-1}) \tag{19}$$

Comparing coefficients in the expansion of the two sides of this equation in powers of λ gives

$$\bar{D}_n = e^{-i\Phi} D_{N-n} \tag{20}$$

The phase is $\Phi = \arg \det(-\mathbf{T}) = 2\pi \mathcal{N}(E)$ where $\mathcal{N}(E)$ is the smoothed level counting function. Using Eq. (20) we see that we may express

$$D = 2e^{i\pi\mathcal{N}} \operatorname{Re} e^{-i\pi\mathcal{N}} \sum_{n=0}^{N_1} D_n = e^{i\pi\mathcal{N}} \Delta \tag{21}$$

[We here and in the future always take $N \equiv 2N_1 + 1$ to be odd. The formulas for even N are similar.] It is convenient to define

$$\tilde{\Delta} = e^{-i\pi\mathcal{N}} \sum_{n=0}^{N_1} D_n \tag{22}$$

so that

$$\Delta(E) = 2 \operatorname{Re} \tilde{\Delta}(E) \tag{23}$$

Thus, only composite orbits of SS length shorter than $N/2$ are needed, since the contribution of orbits between $N/2$ and N are expressed in terms of shorter orbits. This is the phenomenon termed *resurgence* by Berry and Keating,[5] namely, the longer orbits resurge to give the contribution of the short orbits, with an additional, very important, phase. This expression for the *spectral determinant* $\Delta(E)$, which vanishes on the QCA spectrum, and only on the spectrum, is a generalization of the major result of refs. 5, 4, and 6. It is more general in that it does not rely on explicit expressions for the prefactors in the Gutzwiller trace formula, which are typically written down for hard chaos only. Numerical tests have very successfully confirmed the efficacy of Eq. (23).[14]

Note that, even a very simple approximation, such as $\sum_{n=0}^{N_1} D_n \sim 1$ leads to results which are not grossly in error, namely to energy levels spaced with the local mean level spacing. Roughly speaking, one can say that composite classical orbits with n near N, account for the mean level spacing. Short orbits, $n \ll N$, give correlations between levels which are many mean levels spacings apart, while orbits with $n \approx N/2$ contribute random matrix like short range fluctuations and level repulsions.

Remark also that this formulation suggests it may be possible to find energy levels with an error smaller than the mean spacing, [of order h^d in d dimensions, even though errors of order h have been committed in obtaining the D_n's. This is because the zeroes of $\operatorname{Re} \tilde{\Delta}(E)$ come from the zeroes of $\cos(\pi \mathcal{N}(E) - \alpha(E))$ where α is the phase of $\sum_{n=0}^{N_1} D_n$, rather than from the vanishing of $|\sum_{n=0}^{N_1} D_n|$.[15]

VII. RESURGENCE IN THE NUMERATOR FUNCTION

In a similar way, the numerator $\mathbf{N}_m$ displays a resurgence.[7] Taking the Hermitean conjugate of $[\mathbf{1} - \lambda \mathbf{T}]^{-1} = \mathbf{N}/D$ we find

$$\mathbf{N}^\dagger(\lambda) = \frac{\bar{D}(\lambda)}{(\mathbf{1} - \lambda \mathbf{T}^\dagger)} = \frac{-\lambda^{-1} \bar{D}(\lambda)\, \mathbf{T}}{1 - \lambda^{-1} \mathbf{T}} = \frac{-\lambda^{-1} \bar{D}(\lambda)\, \mathbf{T}\mathbf{N}(\lambda^{-1})}{D(\lambda^{-1})}$$

$$= -\lambda^{N-1} e^{-i\Phi} \mathbf{T}\mathbf{N}(\lambda^{-1}) \tag{24}$$

Equating powers of λ, as before, we find that

$$\mathbf{N}_n^\dagger = -e^{-i\Phi} \mathbf{T}\mathbf{N}_{N-n-1} \tag{25}$$

This is the resurgence relation for the numerator operator. Using it we find

$$\mathbf{N} = \sum_{n=0}^{2N_1} \mathbf{N}_n = \sum_{n=0}^{N_1-1} (\mathbf{N}_n - \mathbf{T}^\dagger e^{i\Phi} \mathbf{N}_n^\dagger) + \mathbf{N}_{N_1} \tag{26}$$

It will later be convenient to have *two* powers of $\mathbf{T}^\dagger$ in the resurgent terms rather than one. This is achieved by using the relation

$$\mathbf{N}_n = D_n \mathbf{1} + \mathbf{T}\mathbf{N}_{n-1} \tag{27}$$

Then

$$\mathbf{N} = \sum_{n=0}^{N_1-1} (\mathbf{N}_n - (\mathbf{T}^\dagger)^2 e^{i\Phi} \mathbf{N}_n^\dagger) - \sum_{n=0}^{N_1} \mathbf{T}^\dagger e^{i\Phi} \bar{D}_n \tag{28}$$

VIII. RESURGENCE AND THE WAVE FUNCTIONS

We now apply Eqs. (20) and (25) to a calculation of the energy Green's function. We use Eq. (11) in the QCA. For this, we use expressions for $V_\pm$ in QCA. Thus, for example,

$$V_-(\mathbf{r}, q) = \frac{1}{\sqrt{i\hbar}} \frac{1}{\sqrt{2\pi i\hbar}} \frac{1}{\sqrt{v(\mathbf{r})}} \left| \frac{\partial^2 S(\mathbf{r}, q)}{\partial r_\perp \, \partial q} \right|^{1/2} e^{(i/\hbar) S(\mathbf{r}, q)} \tag{29}$$

Here S is the action of an orbit from the point q on the surface of section to the interior point $\mathbf{r}$, v is the magnitude of the velocity at $\mathbf{r}$. The orbit is assumed to reach $\mathbf{r}$ without crossing the SS after it leaves q. The derivative is with respect to the coordinate perpendicular to the orbit at $\mathbf{r}$.

We now consider $\mathbf{T}^{-1} V_+$ evaluated in the stationary phase approximation. For this we need to find the SΦ point $\bar{q}$ such that $\partial S(\bar{q}, \mathbf{r}')/\partial \bar{q} = \partial S(\bar{q}, q')/\partial \bar{q}$. [See Fig. 2.] This equation implies that q', $\bar{q}$, and $\mathbf{r}'$ all lie on the same orbit, i.e., the orbit from q' to $\bar{q}$ passes through $\mathbf{r}'$. Therefore, we find that $S(\bar{q}, \mathbf{r}') - S(\bar{q}, q') = -S(\mathbf{r}', q')$. The prefactors may be worked out and the result is

$$i \int d\bar{q} \, T^{-1}(q', \bar{q}) \, V_+(\bar{q}, \mathbf{r}') = V_-^\dagger(q', \mathbf{r}') \tag{30}$$

and similarly

$$i \int d\bar{q} \, V_-(\mathbf{r}, \bar{q}) \, T^{-1}(\bar{q}, q) = V_+^\dagger(\mathbf{r}, q) \tag{31}$$

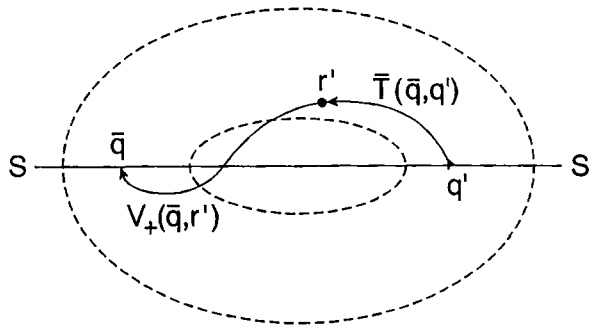

Fig. 2. Schematic of the stationary point $\bar{q}$ which is on the continuation of the orbit from q' to $\mathbf{r}'$.

Using Eq. (28) in Eq. (11), we find that

$$G(\mathbf{r}, \mathbf{r}', E) = G_0(\mathbf{r}, \mathbf{r}', E) + g_L(\mathbf{r}, \mathbf{r}', E) + g_R(\mathbf{r}, \mathbf{r}', E) \tag{32}$$

The first term contains those orbits which do not cross the surface of section in the positive direction. The second g_L is the contribution from longer orbits, going from $\mathbf{r}'$ to $\mathbf{r}$ while crossing the SS some positive number of times. The third term comes originally from the longest contributing orbits, but as we shall see, its contribution is very much like that of the short orbits. This term is

$$g_R \equiv -\frac{\tilde{\Delta}^*}{\Delta} \mathbf{V}_- \mathbf{T}^\dagger \mathbf{V}_+ = i\frac{\tilde{\Delta}^*}{\Delta} \int dq'\, V_+^\dagger(\mathbf{r}, q')\, V_+(q', \mathbf{r}') \tag{33}$$

If $\mathbf{r}$ is not too close to $\mathbf{r}'$, this integral may be performed using stationary phase. There are two stationary points, as shown in Fig. 3, giving contributions

$$g_R = -\frac{\tilde{\Delta}^*}{\Delta}(g_{R1} + g_{R2}) \tag{34}$$

Point q_1 is the first point on the SS encountered by the continuation of the direct orbit from $\mathbf{r}'$ through $\mathbf{r}$. In other words, it is on the continuation of the orbit contributing to G_0. The action at q_1 is $S(q_1, \mathbf{r}') - S(q_1, \mathbf{r}) = S(\mathbf{r}, \mathbf{r}')$, exactly the action that appears in G_0. The prefactors work out to give

$$g_{R1}(\mathbf{r}, \mathbf{r}', E) = G_0(\mathbf{r}, \mathbf{r}', E) \tag{35}$$

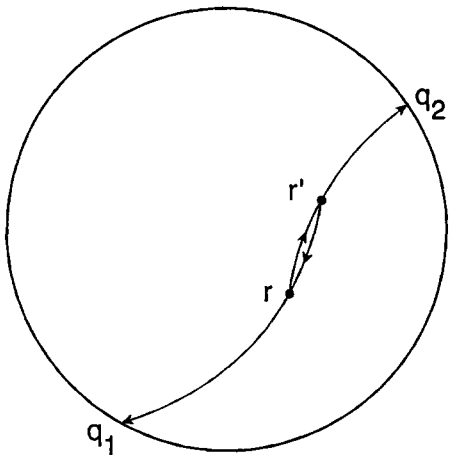

Fig. 3. Illustration of the stationary phase contributions to the integral $\int dq\, V_+^\dagger(\mathbf{r}, q)\, V_+(q, \mathbf{r}')$ for the case of a charged particle in a circular billiard in a perpendicular magnetic field. The two stationary points are labelled q_1 and q_2. This case does not have time reversal invariances.

The other stationary point q_2 is on the SS where the orbit *starting at* $\mathbf{r}$, and passing through $\mathbf{r}'$ first encounters the SS. This leads to an action exponential $e^{-iS(\mathbf{r}', \mathbf{r})/\hbar}$. Working out the prefactors, we find

$$g_{R2}(\mathbf{r}, \mathbf{r}', E) = -G_0^*(\mathbf{r}', \mathbf{r}, E) \tag{36}$$

The expressions for g_{Ri} are in terms of the quasiclassical approximation to G_0. We thus combine G_0 and g_R to give

$$\begin{aligned} g_0(\mathbf{r}, \mathbf{r}', E) + g_0^*(\mathbf{r}', \mathbf{r}, E) &\equiv G_0(\mathbf{r}, \mathbf{r}', E) - \frac{\tilde{\Delta}^*}{\Delta}\left[G_0(\mathbf{r}, \mathbf{r}', E) - G_0^*(\mathbf{r}', \mathbf{r}, E)\right] \\ &= \frac{\tilde{\Delta}}{\Delta} G_0(\mathbf{r}, \mathbf{r}', E) + \frac{\tilde{\Delta}^*}{\Delta} G_0^*(\mathbf{r}', \mathbf{r}, E) \end{aligned} \tag{37}$$

We may similarly express

$$g_L = \sum_{n=1}^{N_1} (g_n + g_n^\dagger) \tag{38}$$

where

$$g_n(\mathbf{r}, \mathbf{r}'; E) = \frac{e^{-i\pi\mathcal{N}}}{\Delta} \iint dq\, dq'\, V_-(\mathbf{r}, q)\, N_{n-1}(q, q')\, V_+(q', \mathbf{r}') \tag{39}$$

Putting this all together, we have the desired formula

$$G(\mathbf{r}, \mathbf{r}', E) = \sum_{n=0}^{N_1} (g_n(\mathbf{r}, \mathbf{r}', E) + g_n^*(\mathbf{r}', \mathbf{r}, E)) \tag{40}$$

There is a similar expression if N is even. Namely, if $N = 2N_1$ the preceding expression applies except that the terms with $n = N_1$ are multiplied by a factor 1/2.

Equation (40) is the **generalization to the Green's function** of the theory for the spectral determinant which is embodied in Eq. (23). It is a *convergent, quasiclassical* expression for the Green's function which can be expressed entirely in terms of classical orbits, when the g_i's are evaluated by stationary phase.

The residue of G at the zeroes of Δ is

$$\Psi_a(\mathbf{r})\, \Psi_a^*(\mathbf{r}') = \sum_{n=0}^{N_1} (g_n'(\mathbf{r}, \mathbf{r}', E_a) + \bar{g}_n'(\mathbf{r}', \mathbf{r}, E_a)) \tag{41}$$

where g_n' is the same as g_n except that the Δ in the denominator is replaced by $\Delta'(E_a) = d\Delta/dE$. This assumes no degeneracy of the energy levels. At present, we don't know exactly how this expression relates to the procedure used by Tomsovic and Heller[16] to obtain semiclassical expressions for wave functions.

It remains to show that the right hand side of Eq. (41) factors into QCA wavefunctions. The integral of Eq. (41) over $\mathbf{r}$, with $\mathbf{r} = \mathbf{r}'$, is unity in QCA. Further, one can show that

$$\int d\bar{\mathbf{r}}\, G(\mathbf{r}, \bar{\mathbf{r}}, E)\, G(\bar{\mathbf{r}}, \mathbf{r}', E) = -\frac{\partial G(\mathbf{r}, \mathbf{r}', E)}{\partial E} \tag{42}$$

for our expression Eq. (40), in QCA, as well as exactly for Eq. (1). These last two properties suffice to show that expression (41) actually *factors*, up to quasiclassically small corrections. To see this, notice that the RHS may be regarded as a self-adjoint operator. Equation (42) shows that this operator is equal to its square, so its eigenvalues are zero or unity The first property shows there is just one unit eigenvalue, which is to say, the RHS of Eq. (41) factors. Thus, Eq. (41) is the **QCA expression for the wave functions.**

IX. SUMMARY

Equation (23) is the best expression known giving the spectrum in the extreme version of the quasiclassical approximation expressed entirely in

terms of classical orbits. It was obtained, under special assumptions on the underlying chaos, in the famous work we cited in the introduction. By use of the Fredholm theory, that work has been extended to the energy Green's function, which in principle contains everything there is to know. Our expression for the energy Green's function in QCA which corresponds to Eq. (23) is Eq. (40). We also obtain an expression, Eq. (41) for the wave functions in terms of classical orbits.

We have not had to make any assumptions on the nature of the chaos or lack thereof in the underlying classical system to obtain these results. Rather, we have had to assume that our surface of section is chosen sufficiently well that the quasiclassical expression $T(q, q', E)$ is a good approximation to the exact kernel $K(q, q', E)$. This requires that the QCA be good for classically rather *short* orbits, [but still long compared with the wavelength], something that is usually relatively easy to accomplish. At this level, there is no difficulty in dealing with mixed chaos. Effects such as diffraction can be accounted for by keeping higher order contributions to T, that is, by including corrections to Eq. (12).

The crucial feature of the Fredholm theory that we have used is the expression of a divergent series by a ratio of absolutely convergent ones. In this way, we have expressed the numerator as a sum over *composite orbits from* $\mathbf{r}'$ to $\mathbf{r}$, in which *ordinary* orbits from $\mathbf{r}'$ to $\mathbf{r}$ are composed with *periodic* orbits. Cancellations result, because a long ordinary orbit passes close to periodic orbits, and so can be approximately decomposed into a shorter ordinary orbit plus periodic ones. These compositions are organized by the *number of surface of section crossings*, and the determinantal structure implies that there are strong cancellations between different contributions, so much so that *only orbits of less than half the Heisenberg time* need be considered.

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Although this work is not statistical in nature, it is appropriate for an issue in tribute to Leo Kadanoff, who has made many contributions to many branches of physics. Fortunately for me, our work has "crossed paths" several times since the almost simultaneous beginnings of our respective careers. I consider it a privilege to know him. The work was partially supported by NSF Grant DMR-9625549.

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