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A direct link between the quantum-mechanical and semiclassical determination of scattering resonances

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Abstract. We investigate the scattering of a point particle from n non-overlapping, disconnected hard disks which are fixed in the two-dimensional plane and study the connection between the spectral properties of the quantum-mechanical scattering matrix and its semiclassical equivalent based on the semiclassical zeta function of Gutzwiller and Voros. We rewrite the determinant of the scattering matrix in such a way that it separates into the product of n determinants of one-disk scattering matrices—representing the incoherent part of the scattering from the n-disk system—and the ratio of two mutually complex conjugate determinants of the genuine multi-scattering kernel, M, which is of Korringa–Kohn–Rostoker-type and represents the coherent multi-disk aspect of the n-disk scattering. Our result is well defined at every step of the calculation, as the on-shell T-matrix and the kernel $\mathsf{M}-\mathbf{1}$ are shown to be trace-class. We stress that the cumulant expansion (which *defines* the determinant over an infinite, but trace-class matrix) induces the curvature regularization scheme to the Gutzwiller–Voros zeta function and thus leads to a new, well defined and direct derivation of the semiclassical spectral function. We show that unitarity is preserved even at the semiclassical level.

1. Introduction

In scattering problems whose classical analogue is completely hyperbolic or even chaotic, as for example n-disk scattering systems, the connection between the spectral properties of exact quantum mechanics and semiclassics has been rather indirect in the past. Mainly the resonance predictions of exact and semiclassical calculations have been compared, which of course still is a useful exercise, but does not fully capture the rich structure of the problem. As shown in [1], there exist several semiclassical spectral functions which predict the very same leading resonances but give different results for the phase shifts. Similar results are known for bound systems, see [2, 3]: the comparison of the analytic structure of the pertinent spectral determinant with various semiclassical zeta functions furnishes the possibility of making much more discriminating tests of the semiclassical approximation than the mere comparison of exact eigenvalues with the corresponding semiclassical predictions.

In the exact quantum-mechanical calculations the resonance poles are extracted from the zeros of a characteristic scattering determinant (see e.g. [4]), whereas the semiclassical predictions follow from the zeros (poles) of a semiclassical spectral determinant (trace)

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of Gutzwiller [5] and Voros [6]. These semiclassical quantities have either been *formally* (i.e. without induced regularization prescription) taken over from bounded problems (where the semiclassical reduction is performed via the spectral density) [7, 8] or they have been extrapolated from the corresponding *classical* scattering determinant [9, 10]. Here, our aim is to construct a *direct* link between the quantum-mechanical and the semiclassical treatment of hyperbolic scattering in a concrete context, the n-disk repellers. The latter belong to the simplest realizations of hyperbolic or even chaotic scattering problems, since they have the structure of a quantum billiard—without any confining (outer) walls. Special emphasis is given to a well defined quantum-mechanical starting point which allows for the semiclassical reduction *including* the appropriate regularization prescription. In this context the word 'direct' refers to a link which is not of *formal* nature, but includes a proper regularization prescription which is *inherited* from quantum mechanics, and not *imposed from the outside by hand*.

The n-disk problem consists in the scattering of a scalar point particle from $n > 1$ circular, non-overlapping, disconnected hard disks which are fixed in the two-dimensional plane. Following the methods of Gaspard and Rice [4] we construct the pertinent on-shell $\mathbf{T}$-matrix which splits into the product of three matrices $\mathbf{C}(k)\mathbf{M}^{-1}(k)\mathbf{D}(k)$. The matrices $\mathbf{C}(k)$ and $\mathbf{D}(k)$ couple the incoming and outgoing scattering wave (of wavenumber k), respectively, to *one* of the disks, whereas the matrix $\mathbf{M}(k)$ parametrizes the scattering interior, i.e. the *multi-scattering* evolution in the multi-disk geometry. The understanding is that the resonance poles of the $n > 1$ disk problem can only result from the zeros of the characteristic determinant $\det \mathbf{M}(k)$; see the quantum mechanical construction of Gaspard and Rice [4] for the three-disk scattering system [11–14]. Their work relates to Berry's application [15, 16] of the Korringa–Kohn–Rostoker (KKR) method [17] to the (infinite) two-dimensional Sinai-billiard problem which in turn is based on Lloyd's multiple scattering method [18, 19] for a finite cluster of non-overlapping muffin-tin potentials in three dimensions.

On the semiclassical side, the geometrical primitive periodic orbits (labelled by p) are summed up—including repeats (labelled by r)—in the Gutzwiller–Voros zeta function [5, 6, 9]

$$Z_{\mathrm{GV}}(z;k) = \exp\left\{-\sum_p \sum_{r=1}^{\infty} \frac{1}{r} \frac{(z^{n_p} t_p(k))^r}{1-(1/\Lambda_p^r)}\right\} \tag{1.1}$$

$$= \prod_p \prod_{j=0}^{\infty} \left(1 - \frac{z^{n_p} t_p(k)}{{\Lambda_p}^j}\right) \tag{1.2}$$

where $t_p(k) = \mathrm{e}^{\mathrm{i}kL_p - \mathrm{i}\nu_p\pi/2}/\sqrt{|\Lambda_p|}$ is the so-called pth cycle, n_p is its topological length and z is a book-keeping variable for keeping track of the topological order. The input is purely geometrical, i.e. the lengths L_p, the Maslov indices ν_p and the stabilities (the leading eigenvalues of the stability matrices) Λ_p of the pth primitive periodic orbits. Note that both expressions for the Gutzwiller–Voros zeta function, the original one (1.1) and the reformulation in terms of an infinite product (1.2), are purely formal. In general, they may not exist without regularization. (An exception is the non-chaotic two-disk system, since it has only one periodic orbit, $t_0(k)$ [20].) Therefore, the semiclassical resonance poles are normally computed from $Z_{\mathrm{GV}}(z = 1; k)$ in the (by hand imposed) curvature expansion [8, 9, 21] up to a given topological length m. This procedure corresponds to a Taylor expansion of $Z_{\mathrm{GV}}(z; k)$ in z around $z = 0$ up to order z^m (with z taken to be one at the end):

$$Z_{\mathrm{GV}}(z;k) = z^0 - z\sum_{n_p=1}\frac{t_p}{1-(1/\Lambda_p)} \tag{1.3}$$

$$-\frac{z^2}{2}\left\{\sum_{n_p=2}\frac{2t_p}{1-(1/\Lambda_p)} + \sum_{n_p=1}\frac{(t_p)^2}{1-(1/\Lambda_p)^2} - \sum_{n_p=1}\sum_{n_{p'}=1}\frac{t_p}{1-(1/\Lambda_p)}\frac{t_{p'}}{1-(1/\Lambda_{p'})}\right\} + \cdots. \tag{1.4}$$

This is one way of regularizing the formal expression of the Gutzwiller–Voros zeta function (1.1). The hope is that the limit $m \to \infty$ exists—at least in the semiclassical regime $\mathrm{Re}\, k \gg 1/a$ where a is the characteristic length of the scattering potential. We will show later that in the quantum-mechanical analogue—the cumulant expansion—this limit can be taken.

As mentioned at the beginning of this paper, the connection between quantum mechanics and semiclassics for these scattering problems has been the comparison of the corresponding resonance poles, the zeros of the characteristic determinant on the one hand and the zeros of the Gutzwiller–Voros zeta function—in general in the curvature expansion—on the other. In the literature (see e.g. [7, 8, 13] based on [22, 23]) this link is motivated by the semiclassical limit of the left-hand sides of the Krein–Friedel–Lloyd sum for the (integrated) spectral density [24, 25] and [18, 19]

$$\lim_{\epsilon\to+0}\lim_{b\to\infty}\left(N^{(n)}(k+\mathrm{i}\epsilon;b) - N^{(0)}(k+\mathrm{i}\epsilon;b)\right) = \frac{1}{2\pi}\mathrm{Im}\,\mathrm{Tr}\ln\mathbf{S}(k) \tag{1.5}$$

$$\lim_{\epsilon\to+0}\lim_{b\to\infty}\left(\rho^{(n)}(k+\mathrm{i}\epsilon;b) - \rho^{(0)}(k+\mathrm{i}\epsilon;b)\right) = \frac{1}{2\pi}\mathrm{Im}\,\mathrm{Tr}\frac{\mathrm{d}}{\mathrm{d}k}\ln\mathbf{S}(k). \tag{1.6}$$

See also [26] for a modern discussion of the Krein–Friedel–Lloyd formula and [23, 27] for the connection of (1.6) to the Wigner time delay. In this way the scattering problem is replaced by the difference of two bounded circular reference billiards of the same radius b which will eventually be taken to infinity, where one contains in its interior the scattering configuration and the other one is empty. Here, $\rho^{(n)}(k;b)$ $(N^{(n)}(k;b))$ and $\rho^{(0)}(k;b)$ $(N^{(0)}(k;b))$ are the spectral densities (integrated spectral densities) in the presence or absence of the scatterers, respectively. In the semiclassical limit, they will be replaced by a smooth Weyl term and an oscillating periodic orbit sum. Note that the above expressions only make sense for wavenumbers k above the real axis. In particular, if k is chosen to be real, ϵ must be greater than zero. Otherwise, the exact left-hand sides would give discontinuous staircase or delta functions, respectively, whereas the right-hand sides are by definition continuous functions of k. Thus, the order of the two limits in (1.5) and (1.6) is important, see, for example Balian and Bloch [22] who stress that smoothed level densities should be inserted into the Friedel sums.

We stress that these links are of *indirect* nature, since unregulated expressions for the semiclassical Gutzwiller trace formula for *bound* systems arise on the left-hand sides of the (integrated) Krein–Friedel–Lloyd sums in the semiclassical reduction. Neither the curvature regularization scheme nor other constraints on the periodic orbit sum follow from this in a natural way. Since the indirect link of (1.5) and (1.6) is made with the help of bound systems, the question might arise, for instance, whether in scattering systems the Gutzwiller–Voros zeta function should be resummed according to Berry and Keating [28] or not. This question is answered by the presence of the iϵ term *and* the second limit. The wavenumber is shifted by the iϵ term from the real axis into the upper complex k-plane. This corresponds to a ‘de-hermitezation’ of the underlying Hamiltonian. The Berry–Keating resummation, which explicitly makes use of the reality of the eigenenergies of a *bound system*, does not apply here. The necessity of $+\mathrm{i}\epsilon$ in the semiclassical calculation can be understood by purely phenomenological considerations: without the $+\mathrm{i}\epsilon$ term there is no reason why one should be able to neglect spurious periodic orbits which solely exist because of the introduction of the confining boundary. The subtraction of the second (empty) reference system helps just in the removal of those spurious periodic orbits which never encounter the scattering region. The ones that do so would still survive the first limit $b \to \infty$, if they were not damped out by the $+\mathrm{i}\epsilon$ term.

The expression for the integrated spectral densities is further complicated by the fact that the ϵ-limit and the integration do not commute either. As a consequence there appears on the left-hand side of (1.5) an (in general) undetermined integration constant.

Independently of this comparison via the Krein–Friedel–Lloyd sums, it was shown in [20] that the characteristic determinant $\det \mathbf{M}(k) = \det(\mathbf{1} + \mathbf{A}(k))$ can be re-arranged via $\mathrm{e}^{\mathrm{Tr}\,\ln(\mathbf{1}+\mathbf{A}(k))}$ in a cumulant expansion and that the semiclassical analogues to the first traces, $\mathrm{Tr}\,(\mathbf{A}^m(k))$ $(m = 1, 2, 3, \ldots)$, contain (including creeping periodic orbits) the sums of all periodic orbits (with and without repeats) of total topological length m. Thus (1.4) should be directly compared with its quantum analogue, the cumulant expansion

$$\det(\mathbf{1} + z\mathbf{A}) = 1 - (-z)\,\mathrm{Tr}[\mathbf{A}(k)] - \frac{z^2}{2}\{\mathrm{Tr}[\mathbf{A}^2(k)] - [\mathrm{Tr}\,\mathbf{A}(k)]^2\} + \cdots. \tag{1.7}$$

The knowledge of the traces is sufficient to organize the cumulant expansion of the determinant

$$\det(\mathbf{1} + z\mathbf{A}) = \sum_{m=0}^{\infty} z^m c_m(\mathbf{A}) \tag{1.8}$$

(with $c_0(\mathbf{A}) \equiv 1$) in terms of a recursion relation for the cumulants (see the discussion of the Plemelj–Smithies formula in the appendix)

$$c_m(\mathbf{A}) = \frac{1}{m}\sum_{k=1}^{m}(-1)^{k+1} c_{m-k}(\mathbf{A})\,\mathrm{Tr}(\mathbf{A}^k) \qquad \text{for } m \geqslant 1. \tag{1.9}$$

In the second paper of [20] the geometrical semiclassical analogues to the first three traces were explicitly constructed for the two-disk problem. The so-constructed geometrical terms correspond exactly (including all prefactors, Maslov indices, and symmetry reductions) to the once, twice or three times repeated periodic orbit that is spanned by the two disks. (Note that the two-disk system has only one classical periodic orbit.) In the meantime, one of us has shown that, with the help of Watson resummation techniques [29, 30] and by complete induction, the semiclassical reduction of the quantum mechanical traces of any non-overlapping $2 \leqslant n < \infty$ disk system (where in addition grazing or penumbra orbits [31, 32] have to be avoided in order to guarantee unique isolated saddle-point contributions) reads as follows [33],

$$(-1)^m\,\mathrm{Tr}\,(\mathbf{A}^m(k)) \xrightarrow{\text{s.c.}} \sum_p \sum_{r>0} \delta_{m,rn_p} n_p \frac{t_p(k)^r}{1 - (1/\Lambda_p)^r} + \text{diffractive creeping orbits} \tag{1.10}$$

where t_p are periodic orbits of topological length n_p with r repeats. The semiclassical reduction (1.10) holds of course only in the case that $\mathrm{Re}\,k$ is big enough compared with the inverse of the smallest length scale. Note that (1.10) does not imply that the semiclassical limit $k \to \infty$ and the cumulant limit $m \to \infty$ commute in general, i.e. that the curvature expansion exists. The factor n_p results from the count of the cyclic permutations of a 'symbolic word' of length n_p which all label the same primary periodic orbit t_p. As the leading semiclassical approximation to $\mathrm{Tr}\,(\mathbf{A}^m(k))$ is based on the replacement of the m sums by m integrals which are then evaluated according to the saddle-point approximation, the qualitative structure of the right-hand side of (1.10) is expected. The non-trivial points are the weights, the phases, and the pruning of ghost orbits which according to [33] follows the scheme presented in [15]. In [34–36] $\hbar$-corrections to the geometrical periodic orbits were constructed, whereas the authors of [37] extended the Gutzwiller–Voros zeta function to include diffractive creeping periodic orbits as well.

By inserting the semiclassical approximation (1.10) of the traces into the exact recursion relation (1.9), one can find a compact expression of the curvature-regularized version of the Gutzwiller–Voros zeta function [8, 9, 21]:

$$Z_{\mathrm{GV}}(z;k) = \sum_{m=0}^{\infty} z^m c_m(\mathrm{s.c.}) \tag{1.11}$$

(with $c_0(\mathrm{s.c.}) \equiv 1$), where the curvature terms $c_m(\mathrm{s.c.})$ satisfy the semiclassical recursion relation

$$c_m(\mathrm{s.c.}) = -\frac{1}{m}\sum_{k=1}^{m} c_{m-k}(\mathrm{s.c.}) \sum_p \sum_{r>0} \delta_{k,rn_p} n_p \frac{t_p(k)^r}{1-(1/\Lambda_p)^r} \qquad \text{for } m \geqslant 1. \tag{1.12}$$

In the following, we construct explicitly a *direct* link between the full quantum-mechanical $\mathbf{S}$-matrix and the Gutzwiller–Voros zeta function in the particular case of n-disk scattering. We will show that *all* necessary steps in the quantum-mechanical description are justified. It is demonstrated that the spectral determinant of the n-disk problem splits uniquely into a product of n incoherent one-disk terms and one coherent genuine multi-disk term which under suitable symmetries separates into distinct symmetry classes. Thus, we have found a well defined starting point for the semiclassical reduction. Since the $\mathbf{T}$-matrix and the matrix $\mathbf{A} \equiv \mathbf{M} - \mathbf{1}$ are trace class matrices (i.e. the sum of the diagonal matrix elements is absolutely converging in any orthonormal basis), the corresponding determinants of the n-disk and one-disk $\mathbf{S}$-matrices and the characteristic matrix $\mathbf{M}$ are guaranteed to exist although they are infinite matrices. The cumulant expansion defines the characteristic determinant and guarantees a finite, unambiguous result. As the semiclassical limit is taken, the defining quantum-mechanical cumulant expansion reduces to the curvature-expansion regularization of the semiclassical spectral function. It will also be shown that unitarity is preserved at the semiclassical level under the precondition that the curvature sum converges or is suitably truncated. In the appendix the trace-class properties of all matrices entering the expression for the n-disk $\mathbf{S}$-matrix will be shown explicitly.

2. Direct link

If one is only interested in spectral properties (i.e. in resonances and not in wavefunctions) it is sufficient to construct the determinant, $\det \mathbf{S}$, of the scattering matrix $\mathbf{S}$. The determinant is invariant under any change of a complete basis representing the $\mathbf{S}$-matrix. (The determinant of $\mathbf{S}$ is therefore also independent of the coordinate system.)

For any non-overlapping system of n-disks (which may even have different sizes, i.e. different disk radii: a_j, $j = 1, \ldots, n$) the $\mathbf{S}$-matrix can be split up in the following way [38] using the methods and notation of Gaspard and Rice [4] (see also [19]):

$$\mathbf{S}^{(n)}_{mm'}(k) = \delta_{mm'} - \mathrm{i}\mathbf{C}^{j}_{ml}(k)\{\mathbf{M}^{-1}(k)\}^{jj'}_{ll'}\mathbf{D}^{j'}_{l'm'}(k) \tag{2.1}$$

where $j, j' = 1, \ldots, n$ (with n finite) label the (n) different disks and the quantum numbers $-\infty < m, m', l, l' < +\infty$ refer to a complete set of spherical eigenfunctions, $\{|m\rangle\}$, with respect to the origin of the two-dimensional plane (repeated indices are, of course, summed over). The matrices $\mathbf{C}$ and $\mathbf{D}$ can be found in Gaspard and Rice [4]; they depend on the origin and orientation of the global coordinate system of the two-dimensional plane and are separable in the disk index j. They parametrize the coupling of the incoming and outgoing scattering wave, respectively, to the jth disk and describe, therefore, the single-disk aspects of the scattering of a point particle from the n disks:

$$\mathbf{C}^j_{ml} = \frac{2\mathrm{i}}{\pi a_j} \frac{J_{m-l}(kR_j)}{H^{(1)}_l(ka_j)} \mathrm{e}^{\mathrm{i}m\Phi_{R_j}} \tag{2.2}$$

$$\mathbf{D}^{j'}_{l'm'} = -\pi a_{j'} J_{m'-l'}(kR_{j'}) J_{l'}(ka_{j'})\, \mathrm{e}^{-\mathrm{i}m'\Phi_{R_{j'}}}. \tag{2.3}$$

Here R_j and Φ_{R_j} denote the distance and angle, respectively, of the ray from the origin in the two-dimensional plane to the centre of the disk j as measured in the global coordinate system. $H^{(1)}_l(kr)$ is the ordinary Hankel function of first kind and $J_l(kr)$ the corresponding ordinary Bessel function. The matrix $\mathbf{M}$ is the genuine multi-disk 'scattering' matrix with eliminated single-disk properties (in the pure one-disk scattering case $\mathbf{M}$ becomes just the identity matrix) [38]:

$$\mathbf{M}^{jj'}_{ll'} = \delta_{jj'}\delta_{ll'} + (1-\delta_{jj'}) \frac{a_j}{a_{j'}} \frac{J_l(ka_j)}{H^{(1)}_{l'}(ka_{j'})} H^{(1)}_{l-l'}(kR_{jj'}) \Gamma_{jj'}(l,l'). \tag{2.4}$$

It has the structure of a KKR matrix (see [15, 16, 19]) and is the generalization of the result of Gaspard and Rice [4] for the equilateral three-disk system to a general n-disk configuration where the disks can have *different* sizes. Here, $R_{jj'}$ is the separation between the centres of the jth and j'th disk and $R_{jj'} = R_{j'j}$. The matrix $\Gamma_{jj'}(l,l') = \mathrm{e}^{\mathrm{i}(l\alpha_{j'j} - l'(\alpha_{jj'}-\pi))}$ contains—besides a phase factor—the angle $\alpha_{j'j}$ of the ray from the centre of disk j to the centre of disk j' as measured in the local (body-fixed) coordinate system of disk j. Note that $\Gamma_{jj'}(l,l') = (-1)^{l-l'}(\Gamma_{j'j}(l',l))^*$. The Gaspard and Rice prefactors, i.e. $(\pi a/2\mathrm{i})$, of $\mathbf{M}$ are rescaled into $\mathbf{C}$ and $\mathbf{D}$. The product $\mathbf{CM}^{-1}\mathbf{D}$ corresponds to the three-dimensional result of Lloyd and Smith for the on-shell $\mathbf{T}$-matrix of a finite cluster of non-overlapping muffin-tin potentials. The expressions of Lloyd and Smith (see (98) of [19] and also Berry's form [15]) at first sight seem to look simpler than ours and the ones of [4] for the three-disk system, as, for example, in $\mathbf{M}$ the asymmetric term $a_j J_l(ka_j)/a_{j'} H^{(1)}_{l'}(ka_{j'})$ is replaced by a symmetric combination, $J_l(ka_j)/H^{(1)}_l(ka_j)$. This form, however, is not of trace-class. Thus, manipulations which are allowed within our description are not necessarily allowed in Berry's and Lloyd's formulation. After a *formal* rearrangement of our matrices we can derive the result of Berry and Lloyd. Note, however, that the trace-class property of $\mathbf{M}$ is lost in this formal manipulation, such that the infinite determinant and the corresponding cumulant expansion converge only conditionally, and not absolutely as in our case.

The l-labelled matrices $\mathbf{S}^{(n)} - \mathbf{1}$, $\mathbf{C}$ and $\mathbf{D}$ as well as the $\{l, j\}$-labelled matrix $\mathbf{M} - \mathbf{1}$ are of 'trace-class' (see the appendix for the proofs). A matrix is called 'trace-class', if, independently of the choice of the orthonormal basis, the sum of the diagonal matrix elements converges absolutely; it is called 'Hilbert–Schmidt' if the sum of the absolute squared diagonal matrix elements converges, see the appendix and Reed and Simon [39, 40] for the definitions and properties of trace-class and Hilbert–Schmidt matrices. Here, we will list only the most important ones: (i) any trace-class matrix can be represented as the product of two Hilbert–Schmidt matrices and any such product is trace-class; (ii) the linear combination of a finite number of trace-class matrices is again trace-class; (iii) the hermitean-conjugate of a trace-class matrix is again trace-class; (iv) the product of two Hilbert–Schmidt matrices or of a trace-class and a bounded matrix is trace-class and commutes under the trace; (v) if $\mathbf{B}$ is trace-class, the determinant $\det(\mathbf{1} + z\mathbf{B})$ exists and is an entire function of z; (vi) the determinant is invariant under unitary transformations. Therefore, for all fixed values of k (except at $k \leqslant 0$ (the branch cut of the Hankel functions) and the countable isolated zeros of $H_m^{(1)}(ka_j)$ and of $\operatorname{Det}\mathbf{M}(k)$) the following operations are mathematically allowed:

$$
\begin{aligned}
\det \mathbf{S}^{(n)} &= \det(\mathbf{1} - \mathrm{i}\mathbf{C}\mathbf{M}^{-1}\mathbf{D}) = \exp \operatorname{tr} \ln(\mathbf{1} - \mathrm{i}\mathbf{C}\mathbf{M}^{-1}\mathbf{D}) \\
&= \exp\left\{ -\sum_{N=1}^{\infty} \frac{\mathrm{i}^N}{N} \operatorname{tr}[(\mathbf{C}\mathbf{M}^{-1}\mathbf{D})^N] \right\} \\
&= \exp\left\{ -\sum_{N=1}^{\infty} \frac{\mathrm{i}^N}{N} \operatorname{Tr}[(\mathbf{M}^{-1}\mathbf{D}\mathbf{C})^N] \right\} \\
&= \exp \operatorname{Tr} \ln(\mathbf{1} - \mathrm{i}\mathbf{M}^{-1}\mathbf{D}\mathbf{C}) = \operatorname{Det}(\mathbf{1} - \mathrm{i}\mathbf{M}^{-1}\mathbf{D}\mathbf{C}) \\
&= \operatorname{Det}[\mathbf{M}^{-1}(\mathbf{M} - \mathrm{i}\mathbf{D}\mathbf{C})] \\
&= \frac{\operatorname{Det}(\mathbf{M} - \mathrm{i}\mathbf{D}\mathbf{C})}{\operatorname{Det}(\mathbf{M})}.
\end{aligned}
\tag{2.5}
$$

In fact,

$$
\det(\mathbf{1} + \mu\mathbf{A}) = \exp\left\{ -\sum_{N=1}^{\infty} \frac{(-\mu)^N}{N} \operatorname{tr}[\mathbf{A}^N] \right\}
$$

is only valid for $|\mu \max \lambda_i| < 1$ where λ_i is the ith eigenvalue of $\mathbf{A}$. The determinant is directly defined through its cumulant expansion (see equation (188) of [40]) which is therefore the analytical continuation of the $\mathrm{e}^{\mathrm{tr}\log}$ representation. Thus the $\mathrm{e}^{\mathrm{tr}\,\log}$ notation should be understood here as a compact abbreviation for the defining cumulant expansion. The capital index L is a multi-index $L = (l, j)$. On the left-hand side of (2.5) the determinant and traces are only taken over small l, on the right-hand side they are taken over multi-indices $L = (l, j)$ (we will use the following convention: $\det \ldots$ and $\operatorname{tr} \ldots$ refer to the $|m\rangle$ space, $\operatorname{Det} \ldots$ and $\operatorname{Tr} \ldots$ refer to the multi-spaces). The corresponding complete basis is now $\{|L\rangle\} = \{|m; j\rangle\}$ which now refers to the origin of the jth disk (for fixed j of course) and not to the origin of the two-dimensional plane any longer. In deriving (2.5) the following facts have been used:

(a) $\mathbf{D}^j$, $\mathbf{C}^j$—if their index j is kept fixed—are of trace-class (see the appendix),

(b) and therefore the product $\mathbf{DC}$—now in the multi-space $\{|L\rangle\}$—is of trace-class as long as n is finite (see property (ii));

(c) $\mathbf{M} - \mathbf{1}$ is of trace-class (see the appendix). Thus the determinant $\operatorname{Det}\mathbf{M}(k)$ exists.

(d) $\mathbf{M}$ is bounded, since it is the sum of a bounded and a trace-class matrix.

(e) $\mathbf{M}$ is invertible everywhere where $\operatorname{Det}\mathbf{M}(k)$ is defined (which excludes a countable number of zeros of the Hankel functions $H_m^{(1)}(ka_j)$ and the negative real k-axis, since there is a branch cut) and non-zero (which excludes a countable number of isolated points in the lower k-plane)—see the appendix for these properties. Therefore, and because of (d), the matrix $\mathbf{M}^{-1}$ is bounded.

(f) $\mathbf{C}\mathbf{M}^{-1}\mathbf{D}$, $\mathbf{M}^{-1}\mathbf{D}\mathbf{C}$ are all of trace-class, since they are the product of bounded times trace-class matrices, and $\operatorname{tr}[(\mathbf{C}\mathbf{M}^{-1}\mathbf{D})^N] = \operatorname{Tr}[(\mathbf{M}^{-1}\mathbf{D}\mathbf{C})^N]$, because such products have the cyclic permutation property under the trace (see properties (ii) and (iv)).

(g) $\mathbf{M} - \mathrm{i}\,\mathbf{D}\mathbf{C} - \mathbf{1}$ is of trace-class because of the rule that the sum of two trace-class matrices is again trace-class (see property (ii)).

Thus all the traces and determinants appearing in (2.5) are well defined, except at the above-mentioned k values. Note that in the $\{|m;j\rangle\}$ basis the trace of $\mathbf{M}-\mathbf{1}$ vanishes trivially because of the $\delta_{jj'}$ terms in (2.4). This does not prove the trace-class property of $\mathbf{M}-\mathbf{1}$, since the finiteness (here vanishing) of $\mathrm{Tr}\,(\mathbf{M}-\mathbf{1})$ has to be shown for every complete orthonormal basis. After symmetry reduction (see later) $\mathrm{Tr}\,(\mathbf{M}-\mathbf{1})$, calculated for any irreducible representation, does not vanish any longer. However, the sum of the traces of all irreducible representations weighted by their pertinent degeneracies still vanishes of course. Semiclassically, this corresponds to the fact that only in the fundamental domain can there exist one-letter 'symbolic words'.

Now, the computation of the determinant of the $\mathbf{S}$-matrix is very much simplified in comparison with the original formulation, since the last term of (2.5) is completely written in terms of closed-form expressions and no longer involves $\mathbf{M}^{-1}$. Furthermore, using the notation of Gaspard and Rice [4], one can easily construct

$$\mathbf{M}^{jj'}_{ll'}-\mathrm{i}\mathbf{D}^{j}_{lm'}\mathbf{C}^{j'}_{m'l'}=\delta_{jj'}\delta_{ll'}\left(-\frac{H^{(2)}_{l'}(ka_{j'})}{H^{(1)}_{l'}(ka_{j'})}\right)-(1-\delta_{jj'})\frac{a_j}{a_{j'}}\frac{J_l(ka_j)}{H^{(1)}_{l'}(ka_{j'})}H^{(2)}_{l-l'}(kR_{jj'})\Gamma_{jj'}(l,l') \tag{2.6}$$

where $H^{(2)}_m(kr)$ is the Hankel function of the second kind. Note that $\{H^{(2)}_m(z)\}^*=H^{(1)}_m(z^*)$. The scattering from a single disk is a separable problem and the $\mathbf{S}$-matrix for the one-disk problem with the centre at the origin reads

$$\mathbf{S}^{(1)}_{ll'}(ka)=-\frac{H^{(2)}_l(ka)}{H^{(1)}_l(ka)}\delta_{ll'}. \tag{2.7}$$

This can be seen by comparison of the general asymptotic expression for the wavefunction with the exact solution for the one-disk problem [38]. Using (2.6) and (2.7) and trace-class properties of $\mathbf{M}-\mathbf{1}$, $\mathbf{M}-\mathrm{i}\mathbf{DC}-\mathbf{1}$ and $\mathbf{S}^{(1)}-\mathbf{1}$ one can easily rewrite the right-hand side of (2.5) as

$$\det\mathbf{S}^{(n)}(k)=\frac{\mathrm{Det}\,(\mathbf{M}(k)-\mathrm{i}\mathbf{D}(k)\mathbf{C}(k))}{\mathrm{Det}\,\mathbf{M}(k)}=\left\{\prod_{j=1}^{n}(\det\mathbf{S}^{(1)}(ka_j))\right\}\frac{\mathrm{Det}\,\mathbf{M}(k^*)^\dagger}{\mathrm{Det}\,\mathbf{M}(k)} \tag{2.8}$$

where now the zeros of the Hankel functions $H^{(2)}_m(ka_j)$ have to be excluded as well. In general, the single disks have different sizes. Therefore, they are labelled by the index j. Note that the analogous formula for the three-dimensional scattering of a point particle from n non-overlapping balls (of different sizes in general) is structurally completely the same [38, 41] (except that the negative k-axis is not excluded since the spherical Hankel functions have no branch cut). In the above calculation the fact that $\Gamma^*_{jj'}(l,l')=\Gamma_{jj'}(-l,-l')$ was used [38]. The right-hand side of equation (2.8) is the starting point for the semiclassical reduction, as every single term is guaranteed to exist. The properties of (2.8) can be summarized as follows.

(1) The product of the n one-disk determinants in (2.8) results from the incoherent scattering where the n-disk problem is treated as n single-disk problems.

(2) The whole expression (2.8) respects unitarity, since $\mathbf{S}^{(1)}$ is unitary by itself (because of $\{H^{(2)}_m(z)\}^*=H^{(1)}_m(z^*)$) and since the quotient on the right-hand side of (2.8) is manifestly unitary.

(3) The determinants on the right-hand side in (2.8) run over the multi-index L. This is the proper form to make the symmetry reductions in the multi-space, for example, for the equilateral three-disk system (with disks of the same size) we have

$$\mathrm{Det}\,\mathbf{M}_{3\text{-disk}}=\det\mathbf{M}_{A1}\det\mathbf{M}_{A2}(\det\mathbf{M}_E)^2 \tag{2.9}$$

and for the two-disk system (with disks of the same size)

$$\mathrm{Det}\,\mathbf{M}_{2\text{-disk}} = \det \mathbf{M}_{A1} \det \mathbf{M}_{A2} \det \mathbf{M}_{B1} \det \mathbf{M}_{B2} \tag{2.10}$$

etc. In general, if the disk configuration is characterized by a finite point symmetry group $\mathcal{G}$, we have

$$\mathrm{Det}\,\mathbf{M}_{n\text{-disk}} = \prod_r (\det \mathbf{M}_{D_r}(k))^{d_r} \tag{2.11}$$

where the index r runs over all conjugate classes of the symmetry group $\mathcal{G}$ and D_r is the rth representation of dimension d_r [38]. (See [42] for notation and [43, 44] for the semiclassical analogue.) A simple check that $\mathrm{Det}\,\mathbf{M}(k)$ has been split up correctly is the power of $H_m^{(1)}(ka_j)$ Hankel functions (for fixed m with $-\infty < m < +\infty$) appearing in the denominator of $\prod_r (\det \mathbf{M}_{D_r}(k))^{d_r}$ which has to be the same as in $\mathrm{Det}\,\mathbf{M}(k)$, which in turn has to be the same as in $\prod_{j=1}^n (\det \mathbf{S}^{(1)}(ka_j))$. Note that on the left-hand side the determinants are calculated in the multi-space $\{L\}$. If the n-disk system is totally symmetric, i.e. none of the disks are special in size and position, the reduced determinants on the right-hand side are calculated in the normal (desymmetrized) space $\{l\}$, however, now with respect to the origin of the disk in the fundamental domain and with ranges given by the corresponding irreducible representations. If some of the n-disk are still special in size or position (e.g. three equal disks in a row [45]), the determinants on the right-hand side refer to a corresponding symmetry-reduced multi-space. This is the symmetry reduction on the exact quantum-mechanical level. The symmetry reduction can be most easily shown if one uses again the trace-class properties of $\mathbf{M} - \mathbf{1} \equiv \mathbf{A}$

$$\begin{aligned}\mathrm{Det}\,\mathbf{M} &= \exp\left\{ -\sum_{N=1}^{\infty} \frac{(-1)^N}{N} \mathrm{Tr}\,[\mathbf{A}^N] \right\} = \exp\left\{ -\sum_{N=1}^{\infty} \frac{(-1)^N}{N} \mathrm{Tr}\,[\mathbf{U}\mathbf{A}^N\mathbf{U}^\dagger] \right\} \\ &= \exp\left\{ -\sum_{N=1}^{\infty} \frac{(-1)^N}{N} \mathrm{Tr}\,[(\mathbf{U}\mathbf{A}\mathbf{U}^\dagger)^N] \right\} = \exp\left\{ -\sum_{N=1}^{\infty} \frac{(-1)^N}{N} \mathrm{Tr}\,[\mathbf{A}_{\mathrm{block}}^N] \right\}\end{aligned}$$

where $\mathbf{U}$ is unitary transformation which makes $\mathbf{A}$ block-diagonal in a suitable basis spanned by the complete set $\{|m; j\rangle\}$. These operations are allowed because of the trace-class property of $\mathbf{A}$ and the boundedness of the unitary matrix $\mathbf{U}$ (see the appendix).

As the right-hand side of equation (2.8) splits into a product of one-disk determinants and the ratio of two mutually complex conjugate genuine n-disk determinants, which are all well defined individually, the semiclassical reduction can be performed for the one-disk and the genuine multi-disk determinants separately. In [33] the semiclassical expression for the determinant of the one-disk $\mathbf{S}$-matrix is constructed in analogous fashion to the semiclassical constructions of [20]:

$$\det \mathbf{S}^{(1)}(ka) \approx \{\mathrm{e}^{-\mathrm{i}\pi N(ka)}\}^2 \frac{\{\prod_{\ell=1}^{\infty}[1 - \mathrm{e}^{-\mathrm{i}2\pi\bar{\nu}_\ell(ka)}]\}^2}{\{\prod_{\ell=1}^{\infty}[1 - \mathrm{e}^{+\mathrm{i}2\pi\nu_\ell(ka)}]\}^2} \tag{2.12}$$

with the creeping term [20, 37]

$$\nu_\ell(ka) = ka + \mathrm{e}^{+\mathrm{i}\pi/3}(ka/6)^{1/3}q_\ell + \cdots = ka + \mathrm{i}\alpha_\ell(ka) + \cdots \tag{2.13}$$

$$\bar{\nu}_\ell(ka) = ka + \mathrm{e}^{-\mathrm{i}\pi/3}(ka/6)^{1/3}q_\ell + \cdots = ka - \mathrm{i}(\alpha_\ell(k^*a))^* + \cdots = [\nu_\ell(k^*a)]^* \tag{2.14}$$

and $N(ka) = (\pi a^2k^2)/4\pi + \cdots$ being the leading term in the Weyl approximation for the staircase function of the wavenumber eigenvalues in the disk interior. From the point of view of the scattering particle the interior domains of the disks are excluded relatively to the free evolution without scattering obstacles (see, e.g. [7]), hence the negative sign in front of the Weyl term. For the same reason, the subleading boundary term has a Neumann structure, although the disks themselves obey Dirichlet boundary conditions. Let us abbreviate the right-hand side of (2.12) for a specified disk j as

$$\det \mathbf{S}^{(1)}(ka_j) \xrightarrow{\text{s.c.}} \{\mathrm{e}^{-\mathrm{i}\pi N(ka_j)}\}^2 \, \frac{\widetilde{Z}_l^{(1)}(k^* a_j)^*}{\widetilde{Z}_l^{(1)}(ka_j)} \frac{\widetilde{Z}_r^{(1)}(k^* a_j)^*}{\widetilde{Z}_r^{(1)}(ka_j)} \tag{2.15}$$

where $\widetilde{Z}_l^{(1)}(ka_j)$ and $\widetilde{Z}_r^{(1)}(ka_j)$ are the *diffractional* zeta functions (here and in the following semiclassical zeta functions *with* diffractive corrections shall be labelled by a tilde) for creeping orbits around the jth disk in the *left*-handed sense and the *right*-handed sense, respectively.

The genuine multi-disk determinant $\mathrm{Det}\,\mathbf{M}(k)$ (or $\det \mathbf{M}_{D_r}(k)$ in the case of symmetric disk configurations) is organized according to the cumulant expansion (1.8) which, in fact, *is* the defining prescription for the evaluation of the determinant of an infinite matrix under the trace-class property. Thus, the cumulant arrangement is automatically imposed onto the semiclassical reduction. Furthermore, the quantum-mechanical cumulants satisfy the Plemelj–Smithies recursion relation (1.9) and can therefore solely be expressed by the quantum-mechanical traces $\mathrm{Tr}\,\mathbf{A}^m(k)$. In [33] the semiclassical reduction of the traces, see equation (1.10), has been derived. If this result is inserted back into the Plemelj–Smithies recursion formula, the semiclassical equivalent of the exact cumulants arise. These are nothing but the semiclassical curvatures (1.12), see [8, 9, 21]. Finally, after the curvatures are summed up according to equation (1.11), it is clear that the the semiclassical reductions of the determinants in (2.8) or (2.11) are the Gutzwiller–Voros spectral determinants (with creeping corrections) in the curvature-expansion regularization. In the case where intervening disks 'block out' ghost orbits [15, 46], the corresponding orbits have to be pruned, see [33]. In summary, we have

$$\mathrm{Det}\,\mathbf{M}(k) \xrightarrow{\text{s.c.}} \widetilde{Z}_{\mathrm{GV}}(k)|_{\text{curv. reg.}} \tag{2.16}$$

$$\det \mathbf{M}_{D_r}(k) \xrightarrow{\text{s.c.}} \widetilde{Z}_{D_r}(k)|_{\text{curv. reg.}} \tag{2.17}$$

where creeping corrections are included in the semiclassical zeta functions. The semiclassical limit of the right-hand side of (2.8) is

$$\begin{aligned}\det \mathbf{S}^{(n)}(k) &= \left\{\prod_{j=1}^{n} \det \mathbf{S}^{(1)}(ka_j)\right\} \frac{\mathrm{Det}\,\mathbf{M}(k^*)^\dagger}{\mathrm{Det}\,\mathbf{M}(k)} \\ &\xrightarrow{\text{s.c.}} \left\{\prod_{j=1}^{n} (\mathrm{e}^{-\mathrm{i}\pi N(ka_j)})^2 \frac{\widetilde{Z}_l^{(1)}(k^* a_j)^*}{\widetilde{Z}_l^{(1)}(ka_j)} \frac{\widetilde{Z}_r^{(1)}(k^* a_j)^*}{\widetilde{Z}_r^{(1)}(ka_j)}\right\} \frac{\widetilde{Z}_{\mathrm{GV}}(k^*)^*}{\widetilde{Z}_{\mathrm{GV}}(k)}\end{aligned} \tag{2.18}$$

where we now suppress the qualifier $\cdots|_{\text{curv. reg.}}$. For systems which allow for complete symmetry reductions (i.e. equivalent disks with $a_j = a \ \forall j$.) the semiclassical reduction reads

$$\begin{aligned}\det \mathbf{S}^{(n)}(k) &= \{\det \mathbf{S}^{(1)}(ka)\}^n \frac{\prod_r \{\det \mathbf{M}_{D_r}(k^*)^\dagger\}^{d_r}}{\prod_r \{\det \mathbf{M}_{D_r}(k)\}^{d_r}} \\ &\xrightarrow{\text{s.c.}} \{\mathrm{e}^{-\mathrm{i}\pi N(ka)}\}^{2n} \left\{\frac{\widetilde{Z}_l^{(1)}(k^* a)^*}{\widetilde{Z}_l^{(1)}(ka)} \frac{\widetilde{Z}_r^{(1)}(k^* a)^*}{\widetilde{Z}_r^{(1)}(ka)}\right\}^n \frac{\prod_r \{\widetilde{Z}_{D_r}(k^*)^*\}^{d_r}}{\prod_r \{\widetilde{Z}_{D_r}(k)\}^{d_r}}\end{aligned} \tag{2.19}$$

in obvious correspondence. (See [43, 44] for the symmetry reductions of the Gutzwiller–Voros zeta function.) These equations do not only give a relation between exact quantum mechanics and semiclassics at the poles, but for *any* value of k in the allowed k region (e.g. $\mathrm{Re}\,k > 0$). There is the caveat that the semiclassical limit and the cumulant limit might not commute in general and that the curvature expansion has a finite domain of convergence [9, 10, 47].

It should be noted that for *bound* systems the idea to focus not only on the positions of the zeros (eigenvalues) of the zeta functions, but also on their analytic structure and their values taken elsewhere has been studied in [2, 3].

3. Discussion

We have shown that (2.8) is a well defined starting point for the investigation of the spectral properties of the exact quantum-mechanical scattering of a point particle from a finite system of non-overlapping disks in two dimensions. The genuine coherent multi-disk scattering decouples from the incoherent superposition of n single-disk problems. We have, furthermore, demonstrated that (2.18) (or, for symmetry-reducible problems, equation (2.19)) closes the gap between the quantum mechanical and the semiclassical description of these problems. Because the link involves determinants of infinite matrices with trace-class kernels, the defining cumulant expansion automatically induces the curvature expansion for the semiclassical spectral function. We have also shown that in n-disk scattering systems unitarity is preserved on the semiclassical level.

The result of (2.18) is compatible with Berry's expression for the integrated spectral density in Sinai's billiard (a *bound* $n \to \infty$ disk system, see equation (6.11) of [15]) and—in general—with the Krein–Friedel–Lloyd sums (1.5). However, all the factors in the first line of the expressions (2.18) and (2.19) are not just of formal nature, but shown to be *finite* except at the zeros of the Hankel functions, $H_m^{(1)}(ka)$ and $H_m^{(2)}(ka)$, at the zeros of the various determinants and on the negative real k-axis, since $\mathbf{M}(k) - \mathbf{1}$ and $\mathbf{S}^{(1)}(k) - \mathbf{1}$ are 'trace-class' almost everywhere in the complex k-plane.

The semiclassical expressions (second lines of (2.18) and (2.19)) are finite, if the zeta functions follow the induced curvature expansion and if the limit $m \to \infty$ exists also semiclassically (the curvature limit $m \to \infty$ and the semiclassical limit $\mathrm{Re}\, k \to \infty$ do not have to commute). The curvature regularization is the semiclassical analogue to the well defined quantum-mechanical cumulant expansion. This justifies the formal manipulations of [7, 8, 48].

Furthermore, even semiclassically, unitarity is automatically preserved in scattering problems (without any reliance on re-summation techniques following Berry and Keating [28] which are necessary and only applicable in bound systems), since

$$\det \mathbf{S}^{(n)}(k)^{\dagger} = \frac{1}{\det \mathbf{S}^{(n)}(k^{*})} \tag{3.1}$$

is valid both quantum mechanically (see the first lines of (2.18) and (2.19)) and semiclassically (see the second lines of (2.18) and (2.19)). There is the caveat that the curvature-regulated semiclassical zeta function has a finite domain of convergence defined by the poles of the dynamical zeta function in the lower complex k-plane [9, 10, 47]. Below this boundary line the semiclassical zeta function has to be truncated at finite order in the curvature expansion [1]. Thus, under the stated conditions unitarity is preserved for n-disk scattering systems on the semiclassical level. On the other hand, unitarity can, therefore, not be used in scattering problems to gain any constraints on the structure of $\widetilde{Z}_{\mathrm{GV}}$ as it could in bound systems, see [28].

To each (quantum-mechanical or semiclassical) pole of $\det \mathbf{S}^{(n)}(k)$ in the lower complex k-plane determined by a zero of $\mathrm{Det}\, \mathbf{M}(k)$, there belongs a zero of $\det \mathbf{S}(k)$ in the upper complex k-plane determined by a zero of $\mathrm{Det}\, \mathbf{M}(k^{*})$ with the same $\mathrm{Re}\, k$ value, but opposite

Im k. We have also demonstrated that the zeta functions of the pure one-disk scattering and the genuine multi-disk scattering decouple, i.e. the one-disk poles do not influence the position of the *genuine* multi-disk poles. However, $\mathrm{Det}\,\mathbf{M}(k)$ does not only possess zeros, but also poles. The latter exactly cancel the poles of the product of the one-disk determinants, $\prod_{j=1}^{n} \det \mathbf{S}^{(1)}(ka_j)$, since both involve the same 'number' and 'power' of $H_m^{(1)}(ka_j)$ Hankel functions in the denominator. The same is true for the poles of $\mathrm{Det}\,\mathbf{M}(k^*)^\dagger$ and the *zeros* of $\prod_{j=1}^{n} \det \mathbf{S}^{(1)}(ka_j)$, since in this case the 'number' of $H_m^{(2)}(ka_j)$ Hankel functions in the denominator of the former and the numerator of the latter is the same—see also Berry's discussion on the same cancellation in the integrated spectral density of Sinai's billiard, equation (6.10) of [15]. Semiclassically, this cancellation corresponds to a removal of the additional creeping contributions of topological length zero, $1/(1-\exp(\mathrm{i}2\pi\nu_\ell))$, from $\widetilde{Z}_{\mathrm{GV}}$ by the one-disk diffractive zeta functions, $\widetilde{Z}_l^{(1)}$ and $\widetilde{Z}_r^{(1)}$. The orbits of topological length zero result from the geometrical sums over additional creepings around the single disks, $\sum_{n_w=0}^{\infty}(\exp(\mathrm{i}2\pi\nu_\ell))^{n_w}$ (see [37]). They multiply the ordinary creeping paths of non-zero topological length. Their cancellation is very important in situations where the disks nearly touch, since in such geometries the full circulations of creeping orbits around any of the touching disks should clearly be suppressed, as it now is. Therefore, it is important to keep a consistent account of the diffractive contributions in the semiclassical reduction. Because of the decoupling of the one-disk from the multi-disk determinants, a direct clear comparison of the quantum mechanical cluster phase shifts of $\mathrm{Det}\,\mathbf{M}(k)$ with the semiclassical ones of the Gutzwiller–Voros zeta function $Z_{\mathrm{GV}}(k)$ is possible. Without the decoupling the cluster phase shifts would be only small modulations on the dominating single-disk phase shifts (see [1, 33]).

In the standard cumulant expansion (see (1.8) with the Plemelj–Smithies recursion formula (1.9)) as well as in the curvature expansion (see (1.11) with (1.12)) there are large cancellations involved which become more and more dramatic the higher the cumulant order is. Let us order—without loss of generality—the eigenvalues of the trace-class operator $\mathbf{A}$ as follows:

$$|\lambda_1| \geqslant |\lambda_2| \geqslant \cdots \geqslant |\lambda_{i-1}| \geqslant |\lambda_i| \geqslant |\lambda_{i+1}| \geqslant \cdots .$$

This is always possible because the sum over the moduli of the eigenvalues is finite for trace-class operators. Then, in the standard (Plemelj–Smithies) cumulant evaluation of the determinant there are cancellations of big numbers, for example, at the lth cumulant order ($l > 3$) all the intrinsically large 'numbers' $\lambda_1^l, \lambda_1^{l-1}\lambda_2, \ldots, \lambda_1^{l-2}\lambda_2\lambda_3, \ldots$ and many more have to cancel out, such that the right-hand side of

$$\det(\mathbf{1} + z\mathbf{A}) = \sum_{l=0}^{\infty} z^l \sum_{j_1<\cdots<j_l} \lambda_{j_1}(\mathbf{A})\cdots\lambda_{j_l}(\mathbf{A}). \tag{3.2}$$

is finally left over. Algebraically, the large cancellations in the exact quantum-mechanical calculation do not matter. However, if the determinant is calculated numerically, large cancellations might spoil the result or even the convergence. Moreover, if further approximations are made as, for example, the transition from the exact cumulant to the semiclassical curvature expansion, these large cancellations might be potentially dangerous. Under such circumstances the underlying (algebraic) absolute convergence of the quantum-mechanical cumulant expansion cannot simply induce the convergence of the semiclassical curvature expansion, since *large* semiclassical 'errors' can completely change the convergence properties.

In summary, the non-overlapping disconnected n-disk systems have the great virtue that—although classically completely hyperbolic and for some systems even chaotic—they are quantum-mechanically *and* semiclassically ‘self-regulating’ and also ‘self-unitarizing’ and still simple enough that the semiclassics can be studied directly, independently of the Gutzwiller formalism, and then compared with the latter.

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Appendix A. Existence of the *n*-disk $\mathbf{S}$-matrix and its determinant

Gaspard and Rice [4] derived in a formal way an expression for the $\mathbf{S}$-matrix for the three-disk repeller. We have used the same techniques in generalizing this result to repellers consisting of n disks of *different* radii [33, 38],

$$\mathbf{S}^{(n)} = \mathbf{1} - \mathrm{i}\mathbf{T} \qquad \mathbf{T} = \mathbf{B}^{j} \cdot \mathbf{D}^{j} \tag{A1}$$

$$\mathbf{C}^{j} = \mathbf{B}^{j'} \cdot \mathbf{M}^{j'j} \tag{A2}$$

$$\mathbf{S}^{(n)} = \mathbf{1} - \mathrm{i}\mathbf{C}^{j} \cdot (\mathbf{M}^{-1})^{jj'} \cdot \mathbf{D}^{j'}. \tag{A3}$$

$\mathbf{S}^{(n)}$ denotes the $\mathbf{S}$-matrix for the n-disk repeller and $\mathbf{B}^{j}$ parametrizes the gradient of the wavefunction on the boundary of the disk j. The matrices $\mathbf{C}$ and $\mathbf{D}$ describe the coupling of the incoming and outgoing scattering waves, respectively, to the disk j and the matrix $\mathbf{M}$ is the genuine multi-disk ‘scattering’ matrix with eliminated single-disk properties. $\mathbf{C}$, $\mathbf{D}$ and $\mathbf{M}$ are given by equations (2.2)–(2.4), respectively. The derivations of the expression for $\mathbf{S}$-matrix (A3) and of its determinant (see section 2) are of purely formal character as all the matrices involved are of infinite size. Here, we will show that the performed operations are all well defined. For this purpose, the trace-class ($\mathcal{J}_1$) and Hilbert–Schmidt ($\mathcal{J}_2$) operators will play a central role.

Trace-class and determinants of infinite matrices. We will briefly summarize the definitions and most important properties for trace-class and Hilbert–Schmidt matrices and operators, and for determinants over infinite-dimensional matrices, [39, 49–52] should be consulted for details and proofs.

An operator $\mathbf{A}$ is called *trace class*, $\mathbf{A} \in \mathcal{J}_1$, if and only if, for every orthonormal basis, $\{\phi_n\}$

$$\sum_n |\langle \phi_n, \mathbf{A}\phi_n \rangle| < \infty. \tag{A4}$$

An operator $\mathbf{A}$ is called *Hilbert–Schmidt*, $\mathbf{A} \in \mathcal{J}_2$, if and only if, for every orthonormal basis, $\{\phi_n\}$

$$\sum_n \|\mathbf{A}\phi_n\|^2 < \infty. \tag{A5}$$

The most important properties of the trace and Hilbert–Schmidt classes can be summarized as (see [39, 50]): (a) $\mathcal{J}_1$ and $\mathcal{J}_2$ are $*$ideals., i.e. they are vector spaces closed under scalar multiplication, sums, adjoints and multiplication with bounded operators; (b) $\mathbf{A} \in \mathcal{J}_1$ if and only if $\mathbf{A} = \mathbf{B}\mathbf{C}$ with $\mathbf{B}, \mathbf{C} \in \mathcal{J}_2$; (c) for any operator $\mathbf{A}$, we have $\mathbf{A} \in \mathcal{J}_2$ if $\sum_n \|\mathbf{A}\phi_n\|^2 < \infty$

for a single basis; (d) for any operator $\mathbf{A} \geqslant 0$, we have $\mathbf{A} \in \mathcal{J}_1$ if $\sum_n |\langle \phi_n, \mathbf{A}\phi_n \rangle| < \infty$ for a single basis.

Let $\mathbf{A} \in \mathcal{J}_1$, then the determinant $\det(\mathbf{1} + z\mathbf{A})$ exists [39, 49–52], it is an entire and analytic function of z and it can be expressed by the *Plemelj–Smithies formula:* define $\alpha_m(\mathbf{A})$ for $\mathbf{A} \in \mathcal{J}_1$ by

$$\det(\mathbf{1} + z\mathbf{A}) = \sum_{m=0}^{\infty} z^m \frac{\alpha_m(\mathbf{A})}{m!}. \tag{A6}$$

Then $\alpha_m(\mathbf{A})$ is given by the $m \times m$ determinant

$$\alpha_m(\mathbf{A}) = \begin{vmatrix} \mathrm{Tr}\,(\mathbf{A}) & m-1 & 0 & \cdots & 0 \\ \mathrm{Tr}\,(\mathbf{A}^2) & \mathrm{Tr}\,(\mathbf{A}) & m-2 & \cdots & 0 \\ \mathrm{Tr}\,(\mathbf{A}^3) & \mathrm{Tr}\,(\mathbf{A}^2) & \mathrm{Tr}\,(\mathbf{A}) & \cdots & 0 \\ \vdots & \vdots & \vdots & \vdots & \vdots \\ \mathrm{Tr}\,(\mathbf{A}^m) & \mathrm{Tr}\,(\mathbf{A}^{(m-1)}) & \mathrm{Tr}\,(\mathbf{A}^{(m-2)}) & \cdots & \mathrm{Tr}\,(\mathbf{A}) \end{vmatrix} \tag{A7}$$

with the understanding that $\alpha_0(\mathbf{A}) \equiv 1$ and $\alpha_1(\mathbf{A}) \equiv \mathrm{Tr}\,(\mathbf{A})$. Thus the cumulants $c_m(\mathbf{A}) \equiv \alpha_m(\mathbf{A})/m!$ (with $c_0(\mathbf{A}) \equiv 1$) satisfy the recursion relation

$$c_m(\mathbf{A}) = \frac{1}{m} \sum_{k=1}^{m} (-1)^{k+1} c_{m-k}(\mathbf{A})\,\mathrm{Tr}\,(\mathbf{A}^k) \qquad \text{for } m \geqslant 1.$$

The most important properties of these determinants are: (i) if $\mathbf{A}, \mathbf{B} \in \mathcal{J}_1$, then $\det(\mathbf{1}+\mathbf{A})\det(\mathbf{1}+\mathbf{B}) = \det(\mathbf{1}+\mathbf{A}+\mathbf{B}+\mathbf{AB}) = \det[(\mathbf{1}+\mathbf{A})(\mathbf{1}+\mathbf{B})] = \det[(\mathbf{1}+\mathbf{B})(\mathbf{1}+\mathbf{A})]$; (ii) if $\mathbf{A} \in \mathcal{J}_1$ and $\mathbf{U}$ unitary, then $\det(\mathbf{U}^\dagger(\mathbf{1}+\mathbf{A})\mathbf{U}) = \det(\mathbf{1}+\mathbf{U}^\dagger\mathbf{A}\mathbf{U}) = \det(\mathbf{1}+\mathbf{A})$; (iii) if $\mathbf{A} \in \mathcal{J}_1$, then $(\mathbf{1}+\mathbf{A})$ is invertible if and only if $\det(\mathbf{1}+\mathbf{A}) \neq 0$; (iv) for any $\mathbf{A} \in \mathcal{J}_1$,

$$\det(\mathbf{1} + \mathbf{A}) = \prod_{j=1}^{N(\mathbf{A})} [1 + \lambda_j(\mathbf{A})] \tag{A8}$$

where here and in the following $\{\lambda_j(\mathbf{A})\}_{j=1}^{N(\mathbf{A})}$ are the eigenvalues of $\mathbf{A}$ counted with algebraic multiplicity ($N(\mathbf{A})$ can be infinite).

Now we can return to the actual problem. The $\mathbf{S}^{(n)}$-matrix is given by (A1). The $\mathbf{T}$-matrix is trace-class on the positive real k-axis ($k > 0$), as it is the product of the matrices $\mathbf{D}^j$ and $\mathbf{B}^j$ which will turn out to be trace-class or, respectively, bounded there (see [39, 40] for the definitions). Again formally, we have used that $\mathbf{C}^j = \mathbf{B}^{j'}\mathbf{M}^{j'j}$ implies the relation $\mathbf{B}^{j'} = \mathbf{C}^j(\mathbf{M}^{-1})^{jj'}$. Thus, the existence of $\mathbf{M}^{-1}(k)$ has to be shown, too—except at isolated poles in the lower complex k-plane below the real k-axis and on the branch cut on the negative real k-axis which results from the branch cut of the defining Hankel functions. As we will prove later, $\mathbf{M}(k) - \mathbf{1}$ is trace-class, except at the above-mentioned points in the k-plane. Therefore, using property (iii), we only have to show that $\mathrm{Det}\,\mathbf{M}(k) \neq 0$ in order to guarantee the existence of $\mathbf{M}^{-1}(k)$. At the same time, $\mathbf{M}^{-1}(k)$ will be proven to be bounded as all its eigenvalues and the product of its eigenvalues are then finite. The existence of these eigenvalues follows from the trace-class property of $\mathbf{M}(k)$ which together with $\mathrm{Det}\,\mathbf{M}(k) \neq 0$ guarantees the finiteness of the eigenvalues and their product [39, 49].

We have normalized $\mathbf{M}$ in such a way that we simply have $\mathbf{B} = \mathbf{C}$ for the scattering from a single disk. Note that the structure of the matrix $\mathbf{C}^j$ does not depend on whether the point particle scatters only from a single disk or from n disks. The functional form (2.2) shows that $\mathbf{C}$ cannot have poles on the real positive k-axis ($k > 0$) in agreement with the structure of the $\mathbf{S}^{(1)}$-matrix (see equation (2.7)). If the origin of the coordinate system is placed at the centre of the disk, the matrix $\mathbf{S}^{(1)}$ is diagonal. In the same basis $\mathbf{C}$ becomes diagonal. One can easily see that $\mathbf{C}$ has no zero eigenvalue on the positive real k-axis and that it will be trace-class. So neither $\mathbf{C}$ nor the one-disk (or for that purpose the n-disk) $\mathbf{S}$-matrix can possess poles or zeros on the real positive k-axis. The statement about $\mathbf{S}^{(n)}$ follows simply from the unitarity of the $\mathbf{S}$-matrix which can be checked easily. The fact that $|\det \mathbf{S}^{(n)}(k)| = 1$ on the positive real k-axis cannot be used to disprove that $\mathrm{Det}\,\mathbf{M}(k)$ could be zero there (see equation (2.8)). However, if $\mathrm{Det}\,\mathbf{M}(k)$ were zero there, this 'would-be' pole must cancel out of $\mathbf{S}^{(n)}(k)$. Looking at formula (A3), this pole has to cancel out against a zero from $\mathbf{C}$ or $\mathbf{D}$ where both matrices are already fixed on the one-disk level. Now, it follows from (A8) that $\mathbf{M}(k)$ (provided that $\mathbf{M} - \mathbf{1}$ has been proven trace-class) has only one chance to make trouble on the positive real k-axis, namely, if at least one of its eigenvalues (whose existence is guaranteed) becomes zero. On the other hand, $\mathbf{M}$ has still to satisfy $\mathbf{C}^j = \mathbf{B}^{j'}\mathbf{M}^{j'j}$. Comparing the left- and right-hand sides of $|\mathbf{C}^j_{mm}(k)| = |\mathbf{B}^{j'}_{ml}\mathbf{M}^{j'j}_{lm}|$ in the eigenbasis of $\mathbf{M}$, and having in mind that $\mathbf{C}^j(k)$ cannot have zero eigenvalue for $k > 0$, one finds a contradiction if the corresponding eigenvalue of $\mathbf{M}(k)$ were zero. Hence $\mathbf{M}(k)$ is invertible on the real positive k-axis, provided, as mentioned now several times, $\mathbf{M}(k) - \mathbf{1}$ is trace-class. From the existence of the inverse relation $\mathbf{B}^{j'} = \mathbf{C}^j(\mathbf{M}^{-1})^{jj'}$ and the to be shown trace-class property of $\mathbf{C}^j$ and the boundedness of $(\mathbf{M}^{-1})^{jj'}$, the boundedness of $\mathbf{B}^j$ follows and therefore the trace-class property of the n-disk $\mathbf{T}$-matrix, $\mathbf{T}^{(n)}(k)$ results, except at the above excluded k-values.

It is left for us to prove:

(a) $\mathbf{M}(k) - \mathbf{1} \in \mathcal{J}_1$ for all k, except at the poles of $H^{(1)}_m(ka_j)$ and for $k \leqslant 0$;

(b) $\mathbf{C}^j(k), \mathbf{D}^j(k) \in \mathcal{J}_1$ with the exception of the same k-values mentioned in (a);

(c) $\mathbf{T}^{(1)}(ka_j) \in \mathcal{J}_1$ (again with the same exceptions as in (a)) where $\mathbf{T}^{(1)}$ is the $\mathbf{T}$-matrix of the one-disk problem;

(d) $\mathbf{M}^{-1}(k)$ does not only exist, but is bounded.

Under these conditions all the manipulations of section 2 (equations (2.5) and (2.8)) are justified and $\mathbf{S}^{(n)}$, as in (2.1), and $\det \mathbf{S}^{(n)}$, as in (2.8), are shown to exist.

Proof of $\mathbf{T}^{(1)}(ka_j)) \in \mathcal{J}_1$. The $\mathbf{S}$-matrix for the jth disk is given by

$$\mathbf{S}^{(1)}_{ml}(ka_j) = -\frac{H^{(2)}_l(ka_j)}{H^{(1)}_l(ka_j)}\delta_{ml}. \tag{A9}$$

Thus $\mathbf{V} \equiv -\mathrm{i}\mathbf{T}^{(1)}(ka_j) = \mathbf{S}^{(1)}(ka_j) - \mathbf{1}$ is diagonal. Hence, we can write $\mathbf{V} = \mathbf{U}|\mathbf{V}|$ where $\mathbf{U}$ is diagonal and unitary, and therefore bounded. What is left to prove is that $|\mathbf{V}| \in \mathcal{J}_1$. We just have to show in a special orthonormal basis (the eigenbasis) that

$$\sum_{l=-\infty}^{+\infty} |\mathbf{V}|_{ll} = \sum_{l=-\infty}^{+\infty} 2\left|\frac{J_l(ka_j)}{H^{(1)}_l(ka_j)}\right| < \infty \tag{A10}$$

since $|\mathbf{V}| \geqslant 0$ by definition (see property (d)). The convergence of this series can be shown easily using the asymptotic formulae for Bessel and Hankel functions for large orders, $\nu \to \infty$, ν real:

$$J_\nu(ka) \sim \frac{1}{\sqrt{2\pi\nu}}\left(\frac{eka}{2\nu}\right)^{\nu} \qquad H^{(1)}_\nu(ka) \sim -\mathrm{i}\sqrt{\frac{2}{\pi\nu}}\left(\frac{eka}{2\nu}\right)^{-\nu} \tag{A11}$$

(see, e.g., [53]). From this equation follows the mathematical justification for the impact parameter (or angular momentum) truncation in the semiclassical resolution of the *single* disks, $|m| \leqslant (e/2)ka$. This limit should not be confused with the truncation in the curvature order resulting from the finite resolution of the repelling set of the n-disk problem, see [1]. Under these asymptotic formulae and the summation of the resulting geometrical series, the trace-class property of $|\mathbf{V}| \in \mathcal{J}_1$ and $\mathbf{S}^{(1)} - \mathbf{1} \in \mathcal{J}_1$ follows immediately. That in turn means that $\det \mathbf{S}^{(1)}(ka_j)$ exists and also that the product $\prod_{j=1}^n \det \mathbf{S}^{(1)}(ka_j) < \infty$ if n is finite (see [39, 49]). Note that the limit $n \to \infty$ does not exist in general.

Proof of $\mathbf{A}(k) \equiv \mathbf{M}(k) - \mathbf{1} \in \mathcal{J}_1$. The determinant of the characteristic matrix $\mathbf{M}(k)$ is defined, if $\mathbf{A}(k) \in \mathcal{J}_1$. In order to show this, we split $\mathbf{A}$ into the product of two operators which—as we will show—are both Hilbert–Schmidt. Then the product is trace-class (see property (b)).

Let, therefore, $\mathbf{A} = \mathbf{E} \cdot \mathbf{F}$ with $\mathbf{A} = \mathbf{M} - \mathbf{1}$ as given in (2.4). In order to simplify the decomposition of $\mathbf{A}$, we choose one of the factors, namely, $\mathbf{F}$, as a diagonal matrix. Let

$$\mathbf{F}_{ll'}^{jj'} = \frac{\sqrt{H_{2l}^{(1)}(k\alpha a_j)}}{H_l^{(1)}(ka_j)} \delta^{jj'} \delta_{ll'} \qquad \alpha > 2. \tag{A12}$$

This ansatz already excludes the zeros of the Hankel functions $H_l^{(1)}(ka_j)$ and also the negative real k-axis (the branch cut of the Hankel functions for $k \leqslant 0$) from our final proof of $\mathbf{A}(k) \in \mathcal{J}_1$. First, we have to show that $\|\mathbf{F}\|^2 = \sum_j \sum_l (\mathbf{F}^\dagger \mathbf{F})_{ll}^{jj} < \infty$. We start with

$$\|\mathbf{F}\|^2 \leqslant \sum_{j=1}^n 2 \sum_{l=0}^\infty \frac{|H_{2l}^{(1)}(k\alpha a_j)|}{|H_l^{(1)}(ka_j)|^2} \equiv \sum_{j=1}^n 2 \sum_{l=0}^\infty \boldsymbol{a}_l. \tag{A13}$$

This expression restricts our proof to n-disk configurations with n *finite*. Using the asymptotic expressions for the Bessel and Hankel functions of large orders (A11) (see, e.g., [53]), it is easy to prove the absolute convergence of $\sum_l \boldsymbol{a}_l$ in the case $\alpha > 2$. Therefore, $\|\mathbf{F}\|^2 < \infty$ and because of property (c) we get $\mathbf{F} \in \mathcal{J}_2$.

We now investigate the second factor $\mathbf{E}$. We have to show the convergence of

$$\|\mathbf{E}\|^2 = \sum_{\substack{j,j'=1 \\ j \neq j'}}^n \left(\frac{a_j}{a_{j'}}\right)^2 \sum_{l,l'=-\infty}^\infty \boldsymbol{a}_{ll'} \qquad \boldsymbol{a}_{ll'} = \frac{|J_l(ka_j)|^2 |H_{l-l'}^{(1)}(kR_{jj'})|^2}{|H_{2l'}^{(1)}(k\alpha a_{j'})|} \tag{A14}$$

in order to prove that also $\mathbf{E} \in \mathcal{J}_2$. Using the same techniques as before, the convergence of $\sum_l \boldsymbol{a}_{ll'}$ for $(1+\epsilon)a_j < R_{jj'}$, $\epsilon > 0$, as well as the convergence of $\sum_{l'} \boldsymbol{a}_{ll'}$ for $\alpha a_{j'} < 2R_{jj'}$, $\alpha > 2$, can be shown. We must of course show the convergence of $\sum_{l,l'} \boldsymbol{a}_{ll'}$ for the case $l, l' \to \infty$ as well. Under the asymptotic behaviour of the Bessel and Hankel functions of large order (A11), it is easy to see that it suffices to prove the convergence of $\sum_{l,l'=0}^\infty b_{ll'}$, where

$$b_{ll'} = \frac{(l+l')^{2(l+l')}}{l^{2l} l'^{2l'}} \left(\frac{a_j}{R_{jj'}}\right)^{2l} \left(\frac{\alpha}{2} \frac{a_{j'}}{R_{jj'}}\right)^{2l'}. \tag{A15}$$

In order to show the convergence of the double sum, we introduce new summation indices (M, m), namely $2M := l + l'$ and $m := l - l'$. Using first Stirling's formula for large powers M and then applying the binomial formula in order to perform the summation over m, the convergence of $\sum_{l,l'=0}^\infty b_{ll'}$ can be shown, provided that $a_j + (\alpha/2)a_{j'} < R_{jj'}$. Under this condition the operator $\mathbf{E}$ belongs to the class of Hilbert–Schmidt operators ($\mathcal{J}_2$).

In summary, this means $\mathbf{E}(\mathbf{k}) \cdot \mathbf{F}(\mathbf{k}) = \mathbf{A}(k) \in \mathcal{J}_1$ for those n-disk configurations for which the number of disks is finite and the disks neither overlap nor touch, and for those values of k which lie neither on the zeros of the Hankel functions $H_m^{(1)}(ka_j)$ nor on the negative real k-axis ($k \leqslant 0$). The zeros of the Hankel functions $H_m^{(2)}(k^* a_j)$ are then automatically excluded, too. The zeros of the Hankel functions $H_m^{(1)}(k\alpha a_j)$ in the definition of $\mathbf{E}$ are cancelled by the corresponding zeros of the same Hankel functions in the definition of $\mathbf{F}$ and they can therefore be removed, i.e. a slight change in α re-adjusts the positions of the zeros in the complex k-plane such that they can always be moved to non-dangerous places.

Proof of $\mathbf{C}^j, \mathbf{D}^j \in \mathcal{J}_1$. The expressions for $\mathbf{D}^j$ and $\mathbf{C}^j$ can be found in (2.3) and (2.2). Both matrices contain—for a fixed value of j—only the information of the single-disk scattering. As in the proof of $\mathbf{T}^{(1)} \in \mathcal{J}_1$, we go to the eigenbasis of $\mathbf{S}^{(1)}$. In that basis both matrices $\mathbf{D}^j$ and $\mathbf{C}^j$ become diagonal. Using the same techniques as in the proof of $\mathbf{T}^{(1)} \in \mathcal{J}_1$, we can show that $\mathbf{C}^j$ and $\mathbf{D}^j$ are trace-class. In summary, we have $\mathbf{D}^j \in \mathcal{J}_1$ for all k as the Bessel functions which define that matrix possess neither poles nor branch cuts. The matrix $\mathbf{C}^j$ is trace-class for almost every k, except at the zeros of the Hankel functions $H_m^{(1)}(ka_j)$ and the branch cut of these Hankel functions on the negative real k-axis ($k \leqslant 0$).

Existence and boundedness of $\mathbf{M}^{-1}(k)$. $\mathrm{Det}\,\mathbf{M}(k)$ exists almost everywhere, since $\mathbf{M}(k) - \mathbf{1} \in \mathcal{J}_1$, except at the zeros of $H_m^{(1)}(ka_j)$ and on the negative real k-axis ($k \leqslant 0$). Modulo these points, $\mathbf{M}(k)$ is analytic. Hence, the points of the complex k-plane with $\mathrm{Det}\,\mathbf{M}(k) = 0$ are isolated. Thus, almost everywhere $\mathbf{M}(k)$ can be diagonalized and the product of the eigenvalues weighted by their degeneracies is finite and non-zero. Hence, where $\mathrm{Det}\,\mathbf{M}(k)$ is defined and non-zero, $\mathbf{M}^{-1}(k)$ exists, it can be diagonalized and the product of its eigenvalues is finite. In summary, $\mathbf{M}^{-1}(k)$ is bounded and $\mathrm{Det}\,\mathbf{M}^{-1}(k)$ exists almost everywhere in the complex k-plane.

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