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The eigenfunction problem in higher dimensions: Exact results

(Wigner transform/Wentzel–Kramers–Brillouin method/integral operator spectrum/integral equations in higher dimensions)

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ABSTRACT **A hermitian integral kernel in N-space may be mapped to a corresponding Hamiltonian in $2N$-space by the Wigner transformation. Linear simplectic transformation on the phase space of the Hamiltonian yields a new kernel whose spectrum is unchanged and whose eigenfunctions follow from an explicit unitary transformation. If an integral kernel has a Wigner transform whose surfaces of constant value are concentric ellipsoids, then the Wigner transform yields exact results to the eigenfunction problem. Such behavior is asymptotically generic near extrema of the Wigner transform, from which follow simple and robust asymptotic results for the ends of the eigenvalue spectrum and for the corresponding eigenfunctions.**

It has been shown in ref. 1 that WKB (Wentzel–Kramers–Brillouin) theory [usually presented for differential operators and culminating in the EBK (Einstein–Brillouin–Keller) (2–4) formulas] extends in a useful way to the general eigenfunction problem

$$\int K\{\mathbf{x}, \mathbf{y}\}\psi(\mathbf{y})d\mathbf{y} = \lambda\psi(\mathbf{x}). \quad [1]$$

The formal treatment applies to formal hermitian kernels

$$K\{\mathbf{x}, \mathbf{y}\} = K(\varepsilon(\mathbf{x} + \mathbf{y})/2, \mathbf{x} - \mathbf{y}) = K^*(\varepsilon(\mathbf{x} + \mathbf{y}), \mathbf{y} - \mathbf{x}) \quad [2]$$

for which the integral in Eq. 1 is defined in some sense. Integral, differential, and pseudo-differential operators are included in this class. The results, which are presented as general in following sections, likewise hold for this broad set of operators.

The treatment in ref. 1 begins with the representation of the solution in the form

$$\psi(\mathbf{x}) = \exp[i\phi(\varepsilon\mathbf{x}:\varepsilon)/\varepsilon]. \quad [3]$$

Under the limit $\varepsilon \downarrow 0$ it was seen that the solution of Eq. 1 follows from the properties of the Wigner transform of K,

$$\tilde{K}(\mathbf{q}, \mathbf{p}) = W[K] = \int K(\mathbf{q}, \mathbf{u})\exp(-i\mathbf{p}\cdot\mathbf{u})d\mathbf{u}. \quad [4]$$

It follows directly from hermiticity Eq. **2** *that* $\tilde{K}$ *is real.* Next if we let

$$\mathbf{p} = \lim_{\varepsilon\to 0} \nabla\phi \quad [5]$$

in Eq. **4**, then in the limit equation [1] with Eq. **4** substituted becomes

$$\tilde{K}(\mathbf{q}, \nabla\phi) = \lambda, \quad [6]$$

a partial differential equation for ϕ that bears the same relationship to Eq. **1** that the eiconal equation of geometrical optics (5) bears to the wave operator. The eiconal equation is in fact just an example of our more general case.

Although Eq. **6** results from the lowest order of a formal asymptotic theory no information about the original problem (Eq. **1**) is lost in the limit process indicated in Eq. **5**. In fact the exact kernel is recovered by inverse transform,

$$W^{-1}[\tilde{K}] = K((\mathbf{x} + \mathbf{y})/2, \mathbf{x} - \mathbf{y})$$
$$= \frac{1}{(2\pi)^N}\int K((\mathbf{x} + \mathbf{y})/2, \mathbf{p})\exp[i\mathbf{p}(\mathbf{x} - \mathbf{y})]d\mathbf{p}. \quad [7]$$

(In Eq. **7** and in what follows ε is set to unity.) This observation is underscored by a variety of exact results obtained below, which follow directly from study of $\tilde{K}$. Certain of these results have been reported for the one-dimensional case (7).

Operator Composition

The results given in this section, which will be used later, are all elementary to derive and do not depend on whether the spectrum of a kernel is discrete, continuous, or mixed.

If we write operator composition or product as

$$(\mathrm{K}_1\mathrm{K}_2)\{\mathbf{x}, \mathbf{y}\} = \int \mathrm{K}_1\{\mathbf{x}, \mathbf{z}\}\mathrm{K}_2\{\mathbf{z}, \mathbf{y}\}d\mathbf{z}, \quad [8]$$

then

$$Tr\ \mathrm{K}_1\mathrm{K}_2 = \int \mathrm{K}_1\{\mathbf{x}, \mathbf{z}\}\mathrm{K}_2\{\mathbf{z}, \mathbf{x}\}d\mathbf{z}d\mathbf{x}$$
$$= \frac{1}{(2\pi)^N}\int \tilde{\mathrm{K}}_1(\boldsymbol{\xi})\tilde{\mathrm{K}}_2(\boldsymbol{\xi})d\boldsymbol{\xi}, \quad [9]$$

where

$$\boldsymbol{\xi} = (\mathbf{q}, \mathbf{p}) \quad [10]$$

is the phase space variable.

An immediate corollary is that

$$\int K\{\mathbf{x}, \mathbf{x}\}d\mathbf{x} = \frac{1}{(2\pi)^N}\int \tilde{K}(\boldsymbol{\xi})d\boldsymbol{\xi}, \quad [11]$$

gotten by taking one of the operators of Eq. **9** to be the delta function $\delta(\mathbf{x} - \mathbf{y})$. Note that Eq. **11** may be divergent.

The Wigner transform of an operator product is the bilinear form given by

$$W[\mathrm{K}_1\mathrm{K}_2] \stackrel{def}{=} \tilde{\mathrm{K}}_1 \otimes \tilde{\mathrm{K}}_2$$
$$= \int d\boldsymbol{\xi}^1 d\boldsymbol{\xi}^2 \tilde{\mathrm{K}}_1(\boldsymbol{\xi}^1)\tilde{\mathrm{K}}_2(\boldsymbol{\xi}^2)exp[2i\Delta(\boldsymbol{\xi}^1, \boldsymbol{\xi}^2, \boldsymbol{\xi})], \quad [12]$$

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Abbreviation: EBK, Einstein–Brillouin–Keller.

with

$$\Delta(\xi^1, \xi^2, \xi) = \sum_{k=1}^{N} \begin{vmatrix} q_k^1 - q_k & q_k^2 - q_k \\ p_k^1 - p_k & p_k^2 - p_k \end{vmatrix}. \quad [13]$$

The proof of Eq. **12** is a direct extension of that given in ref. 7. Note each term of the sum **[13]** represents the projected area of the parallelogram generated by the tips of (ξ^1, ξ^2, ξ) in the (q_k, p_k) plane. An alternative representation of **[13]** is

$$\Delta(\xi^1, \xi^2, \xi) = (\xi^1 - \xi) \cdot \mathbf{J} \cdot (\xi^2 - \xi), \quad [14]$$

where **J** is the $2N \times 2N$ antisymmetric matrix

$$J = \begin{bmatrix} 0 & 1 \\ -1 & 0 \end{bmatrix}. \quad [15]$$

It proves convenient to restate the eigenvalue problem (Eq. **1**) in terms of the projection operator based on the eigenfunctions of Eq. **1**,

$$E\{\mathbf{x}, \mathbf{y}\} = \psi(\mathbf{x})\psi^*(\mathbf{y}). \quad [16]$$

The Wigner transform corresponding to Eq. **16** is

$$W[E] = \tilde{E}(\xi) = \tilde{E}(\mathbf{q}, \mathbf{p})$$
$$= \int d\mathbf{u}\psi(\mathbf{q} + \mathbf{u}/2)\psi^*(\mathbf{q} - \mathbf{u}/2)\exp(-i\mathbf{p} \cdot \mathbf{u}). \quad [17]$$

Since

$$KE = \lambda E, \quad [18]$$

it follows from Wigner transformation that

$$\tilde{K} \otimes \tilde{E} = \lambda \tilde{E}. \quad [19]$$

An Isospectral Class of Operators

Consider for the moment two one-dimensional hermitian operators K_1 and K_2. Their Wigner transforms $\tilde{K}_1$ and $\tilde{K}_2$ are therefore real, and we consider level curves

$$\tilde{K}_1(q, p) = \lambda = \tilde{K}_2(q', p')$$

on the (q, p) and (q', p') planes indexed by the level variable, λ. If for all real λ that lead to such curves, these curves enclose equal areas respectively on the (q, p) and (q', p') planes, then asymptotically ($\varepsilon \downarrow 0$ in Eq. **2**) the eigenvalue spectra of K_1 and K_2 are equal (6, 8). (Beyond a value of λ at which the enclosed area goes to infinity the spectrum becomes continuous.) As a consequence of the discussion in ref. 1 we can make a similar remark for the higher dimensional case. If two (real) Wigner transforms $\tilde{K}_1$ and $\tilde{K}_2$, viewed as Hamiltonians, are completely integrable (9) and for equal "energies," λ, have equal sets of action integrals

$$J_k = \oint_{\Upsilon_k} \mathbf{p} \cdot d\mathbf{q}, \quad [20]$$

over their respective irreducible circuits, Υ_k, then asymptotically the corresponding operators K_1 and K_2 will have equal eigenvalue spectra. This is a direct consequence of the EBK formula (6, 8, 9) discussed in ref. 1. (A part of the fine print is the assumption that both Hamiltonians give rise to like caustic structures.) For sets of operators whose corresponding Hamiltonians are connected by linear symplectic transformations, this asymptotic result is exact. This we show next.

For this purpose consider the matrices **M** defined as symplectic by the condition (10)

$$\mathbf{M\, J\, M} = \mathbf{J}. \quad [21]$$

These define linear canonical transformations in the sense of Hamiltonian mechanics:

$$\xi = \mathbf{M}\, \hat{\xi}. \quad [22]$$

Each of these transformations in turn induces a transformation of K to K_M defined through

$$\tilde{K}_M = \tilde{K}(M\hat{\xi}) = \tilde{K}_M(\hat{\xi}). \quad [23]$$

Because Eq. **22** is canonical it leaves the actions, J_k, given by Eq. **20** invariant and therefore from the EBK conditions K_M and K asymptotically as $\varepsilon \downarrow 0$ have the same eigenvalues. However, more can be said:

Under all linear symplectic mappings $\mathrm{K_M}$ *of the operator* K, *as in Eq.* **23**, *every eigenvalue* λ *is exactly invariant,*

$$\mathrm{K_M E_M} = \lambda \mathrm{E_M}. \quad [24]$$

To prove this assertion we introduce Eq. **22** into Eq. **19** to obtain

$$(\tilde{K} \otimes \tilde{E})(M\hat{\xi}) = \lambda\tilde{E}(\mathbf{M}\hat{\xi}) = \lambda\tilde{E}_M(\hat{\xi}). \quad [25]$$

Then if Eq. **12** is applied to the left-hand side of Eq. **25**, with the variable changes $\xi^1 = \mathbf{M}\hat{\xi}^1$, $\xi^2 = \mathbf{M}\hat{\xi}^2$ we obtain [using Eqs. **14** and **21** and det(**M**) = 1]

$$\tilde{K}_M \otimes \tilde{E}_M = \lambda\tilde{E}_M. \quad [26]$$

Finally, if we apply the inverse Wigner transform to Eq. **26** we get Eq. **24**.

It is worth noting that, although the motivation for this observation rests on the invariance of the EBK conditions, which in turn depend on the complete integrability of $\tilde{K}(\xi)$ (as a Hamiltonian) this property plays no role in the proof. The symplectic matrices **M** induce on the operators K isospectral equivalence classes $\{K_M\}$, independently of the Hamiltonian structure of $\tilde{K}_M(\xi)$. Also note the proof is elementary and independent of whether the spectrum is discrete, mixed, or continuous.

Eigenfunction Transformation Under Symplectic Mapping

The eigenfunction transformation under Eq. **23** may be given an explicit form. To show this we express a symplectic matrix in block form

$$\mathbf{M} = \begin{bmatrix} \boldsymbol{\alpha} & \boldsymbol{\beta} \\ \boldsymbol{\Upsilon} & \boldsymbol{\delta} \end{bmatrix}, \quad [27]$$

where each submatrix is $N \times N$. It then follows that:

If ψ_M *denotes an eigenfunction of the transformed kernel, Eq.* **23**,

$$\mathrm{K_M}\psi_\mathrm{M} = \lambda\psi_\mathrm{M} \quad [28]$$

and ψ *represents the corresponding eigenfunction of* K, *then*

$$\psi_\mathrm{M}(\mathbf{x}) = \frac{1}{(2\pi)^{N/2}} \int \frac{d\mathbf{y}\psi(\mathbf{y})}{(\omega\, det(\mathbf{Y}))^{1/2}}$$
$$\times\, exp[-i(\mathbf{x}\mathbf{Y}^{-1}\boldsymbol{\delta}\mathbf{x} - 2\mathbf{x}\mathbf{Y}^{-1}\boldsymbol{\delta}\mathbf{y} + \mathbf{y}\boldsymbol{\alpha}\mathbf{Y}^{-1}\mathbf{y})/2], \quad [29]$$

ω represents a constant of unit magnitude up to which Eq. **29** *is undetermined.*

The somewhat lengthy proof of Eq. **29** is elementary and independent of the details of K and of its spectrum and roughly follows the one-dimensional case.

Eq. **29** *may be shown to be a unitary transformation on ψ, say $\psi_M = U_M\psi$. In this format $K_M = U_M K U_M^{-1}$ from which the isospectral character of the transformation is direct.*

A particularly interesting illustration of these results follows from the one-parameter subgroup of symplectic matrices,

$$\mathbf{M} = \exp(\mathbf{A}t). \qquad [30]$$

Then it may be seen that as a result of the symplectic condition **[21]** the infinitesimal generator **A** must have the form

$$A = \begin{bmatrix} \mathbf{a} & \mathbf{b} \\ \mathbf{c} & -\mathbf{a}^{\dagger} \end{bmatrix}. \qquad [31]$$

with symmetric $N \times N$ submatrices,

$$\mathbf{b} = \mathbf{b}^{\dagger},\ \mathbf{c} = \mathbf{c}^{\dagger}. \qquad [32]$$

The symplectic matrix **[30]** can be thought of as inducing a flow in ξ-space. In fact the flow vector field is given by the Hamiltonian equations of the quadratic Hamiltonian,

$$H = \frac{1}{2}\,\xi \begin{bmatrix} -\mathbf{c} & \mathbf{a}^{\dagger} \\ \mathbf{a} & \mathbf{b} \end{bmatrix} \xi. \qquad [33]$$

Under this flow the eigenfunction (Eq. **29**) becomes a function of t and we write

$$\Psi(\mathbf{x}, t) = \psi_M(\mathbf{x}). \qquad [34]$$

For example by direct calculation it may be shown that Ψ satisfies

$$i\frac{\partial \Psi}{\partial t} = \frac{c_{mn}}{2}\frac{\partial^2 \Psi}{\partial x_m \partial x_n} + \frac{b_{mn}}{2} x_m x_n \Psi - \frac{i}{2} a_{mn}\left(x_m \frac{\partial}{\partial x_n} + \frac{\partial}{\partial x_n} x_m\right)\Psi = G_A \Psi \qquad [35]$$

(repeated indices summed, here and below), where the dependence of the second-order differential operator G_A on **A** is through the submatrices (Eq. **31**). It follows from Eq. **35** that the set of second-order differential operators G_A are infinitesimal generators algebraically isomorphic to the set of matrices **A**. The Green's operator for Eq. **35** is the unitary operator given in integral form by Eq. **29**.

Exactly Solvable Operators

If the Wigner transform of an operator has the form

$$\tilde{K} = \tilde{K}(q_1^2 + p_1^2, q_2^2 + p_2^2, \ldots, q_N^2 + p_N^2) \qquad [36]$$

(or if it can be put into this form by a linear symplectic transformation), then the operator is explicitly solvable. The corresponding kernel,

$$K(\mathbf{q}, \mathbf{x} - \mathbf{y}) = \frac{1}{(2\pi)^N}\int \tilde{K}(q_1^2 + p_1^2, \ldots, q_N^2 + p_N^2)\, \exp(i\mathbf{p}\cdot(\mathbf{x} - \mathbf{y}))d\mathbf{p} \qquad [37]$$

has eigenfunctions

$$\psi = H_{n_1}(x_1)H_{n_2}(x_2)\ldots H_{n_N}(x_N)\exp(-\mathbf{x}^2/2), \qquad [38]$$

where $H_n(x)$ *represents the Hermite polynomial of index* n *(11). The corresponding eigenvalue is given by*

$$\lambda = (-)^{n_1+\ldots+n_N}\int \tilde{K}(r_1, \ldots, r_N)L_{n_1}(2r_1)\ldots L_{n_N}(2r_N)\exp(-r_1 - \ldots - r_N)dr_1 \ldots dr_N, \qquad [39]$$

where L_n *refers the Laguerre polynomial of index* n *(11).*

The proof of these assertions follows the lines of the one-dimensional treatment (7). The steps are elementary and not constrained by the way $\tilde{K}$ in Eq. **36** depends on its arguments except for the permissive condition that the integral Eq. **39** should converge.

Viewed as a Hamiltonian, Eq. **36** is completely integrable and represents a system of separable (generally nonlinear) mechanical oscillators. The actions are given by $J_k = (q_k^2 + p_k^2)/2$ and the corresponding frequencies by $\omega_k = \partial\tilde{K}/\partial J_k$. As an illustration of a case in which such an operator arises, consider the Schrodinger operator G_A that appears in Eq. **35**. Its Wigner transform is the Hamiltonian (Eq. **33**). If the matrix **A** (Eq. **31**) has the generic feature of eigenvalues that occur in imaginary pairs ($\pm i\omega$), the Hamiltonian (Eq. **33**) can be reduced to the form Eq. **36**, and it follows that the eigenfunctions of G_A are products of Hermite functions as in Eq. **38**. [The precise form is complicated by the unraveling of the symplectic form needed to place H (Eq. **33**) in the form of Eq. **36**.]

Although Eq. **36** signifies a separable mechanical problem it does not imply that the corresponding kernel is factorable. As an illustration of this remark consider the 3-space kernel

$$K\{\mathbf{x}, \mathbf{y}\} = \frac{\exp[-|\mathbf{x} - \mathbf{y}|(1 + k^2(\mathbf{x} + \mathbf{y})^2/4)^{1/2}]}{4\pi|\mathbf{x} - \mathbf{y}|}. \qquad [40]$$

The Wigner transform of Eq. **40** is

$$\tilde{K} = \frac{1}{1 + k[(\mathbf{p}/(k)^{1/2})^2 + ((k)^{1/2}\mathbf{q})^2]} \qquad [41]$$

and the operator is thus solvable by the above procedures. In particular, the eigenfunctions are given by Eq. **38** and the eigenvalue calculation, which is given by Eq. **39**, may be reduced to

$$\lambda_{n_1 n_2 n_3} = \frac{1}{k}\int_0^{\infty}\left(\frac{1 - t}{1 + t}\right)^{n_1+n_2+n_3}\frac{\exp(-t/k)}{(1 + t)^3}\,dt. \qquad [42]$$

Under the limit $k \downarrow 0$ it may be shown that

$$\lambda_{n_1 n_2 n_3} \sim \frac{1}{(1 + k(2n_1 + 2n_2 + 2n_3 + 3))}, \qquad [43]$$

a result that is uniform in the subscripts n_1, n_2, n_3. (It should be noted that Eq. **43** is exactly the result given by Eq. **41** if the area rule of the previous paper is applied.) For $k = 0$ the spectrum of Eq. **40** is the continuous interval (0, 1) and Eq. **43** indicates the way in which this is filled in under the limit $k \downarrow 0$.

Principal Eigenfunctions

A significant application of the section above relates the eigenvalue spectrum of a general K to the behavior of $\tilde{K}$ in the neighborhood of one of its extreme points. By ref. 1, this neighborhood corresponds to the extreme eigenvalues in the spectrum of the operator and plays a basic role because it describes modes that are most persistent or most highly amplified. In the neighborhood of an extremal point (after a trivial change of origin) we have

$$\bar{K} \sim \bar{K}^0 + \frac{1}{2}\, \xi_i \xi_j \bar{K}^0_{ij}. \quad \textbf{[44]}$$

This takes us back to the case of a quadratic Hamiltonian, which can be put into the form of Eq. **36** by linear canonical transformation. The approximate eigenfunctions are therefore products of Hermite functions and the eigenvalues follow easily from the methods of the previous section (a simple explicit expression results in this case). In this same vein, higher-order approximations may be achieved by taking Eq. **44** beyond second order and then developing the Hamiltonian in Birkhoff normal form (12, 13).

We comment further that if $\bar{K}$ is not self-adjoint, the "origin" (a singular point of Hamilton's equations) to which we shift to obtain Eq. **44** may lie at a complex point in the (**q**, **p**) phase space, at which the analytic continuation of $\bar{K}$ has a saddle. In particular cases of this sort the procedures summarized above are still effective in calculating the generally complex spectrum.

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