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The eigenfunction problem in higher dimensions: Asymptotic theory

(Wigner transform/WKB method)

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ABSTRACT **The spectral problem for linear operators on fully infinite domains is considered. A transformation first introduced by Wigner is used to show a number of asymptotic results. The method leads to a WKB (Wentzel–Kromers–Brillouin) theory for operators in more than one dimension. This includes practical tools for the approximate evaluation of spectra and eigenfunctions. Several general examples are developed.**

In a fully infinite N-dimensional space, with typical points $\mathbf{x}$ and $\mathbf{y}$, the spectral problem is stated by

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

with eigenvalues λ and eigenfunctions $\psi(\mathbf{x})$. Without being specific the integral in Eq. **1** is regarded as defined in some general sense. Included in the definition are differential operators. For example, the Schrodinger operator is given by the kernel,

$$K\{\mathbf{x}, \mathbf{y}\} = -\frac{1}{2}\nabla^2(\delta(\mathbf{x} - \mathbf{y})) + V([\mathbf{x} + \mathbf{y}]/2)\delta(\mathbf{x} - \mathbf{y}). \qquad [2]$$

In terms of mean and relative positions the kernel becomes

$$K\{\mathbf{x}, \mathbf{y}\} = K((\mathbf{x} + \mathbf{y})/2, (\mathbf{x} - \mathbf{y})). \qquad [3]$$

The eigenvalue problem is now recast as a special case ($\varepsilon = 1$) of the general problem

$$\int d\mathbf{y}\, K(\varepsilon(\mathbf{x} + \mathbf{y})/2, \mathbf{x} - \mathbf{y})\psi(\mathbf{y}; \varepsilon) = \lambda\psi(\mathbf{x}; \varepsilon), \qquad [4]$$

for which asymptotic results in small ε may be developed. If in some sense K depends "gently" on the first argument of Eq. **3**, the asymptotic results yield an approximation when $\varepsilon = 1$.

Alternative formulations of Eq. **4** are given by

$$\int d\mathbf{y}\, K((\mathbf{x} + \mathbf{y})/2, (\mathbf{x} - \mathbf{y})/\varepsilon)\psi(\mathbf{y}; \varepsilon) = \lambda'\psi \qquad [5]$$

and

$$\int d\mathbf{y}\, K(\sqrt{\varepsilon}(\mathbf{x} + \mathbf{y})/2, (\mathbf{x} - \mathbf{y})/\sqrt{\varepsilon})\psi(\mathbf{y}; \sqrt{\varepsilon}) = \lambda''\psi, \qquad [6]$$

where $\lambda = \varepsilon^N\lambda' = \varepsilon^{N/2}\lambda''$, with related transformations of the dependent variables and eigenfunctions. Each such formulation has formal features that make it attractive. Thus Eq. **4** brings out the slow dependence on the first argument, Eq. **5** brings out the peakiness in the second argument, and Eq. **6** incorporates both these features. In adopting Eq. **4** as our starting point we follow an earlier convention (1–3). In what follows, we refer to the first variables of Eq. **3** as "slow," the second as "fast," and when convenient refer to Eq. **3** as a peaking function of its second argument.

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Asymptotic Development

If ε is set to zero in Eq. **4** the kernel becomes translationally invariant in its second argument. This suggests that the eigenfunctions be developed in WKB (Wentzel–Kromers–Brillouin) form [a procedure usually associated with differential operators (4, 5)]

$$\psi_m = A_m(\varepsilon\mathbf{x}; \varepsilon)\exp[i\Phi_m(\varepsilon\mathbf{x})/\varepsilon] = \exp[i\phi_m(\varepsilon\mathbf{x}; \varepsilon)/\varepsilon]. \qquad [7]$$

(Each of the two equivalent forms proves to be useful in the following.) The subscript m in Eq. **7** signifies that a number of branches can be expected, and the solution to Eq. **4** will be in the form of a sum of terms of the form of Eq. **7** (6, 7).

The subscript in Eq. **7** will be suppressed until necessary. The variable change

$$\mathbf{q} = \varepsilon\mathbf{x}, \qquad \mathbf{u} = \mathbf{x} - \mathbf{y} \qquad [8]$$

in Eq. **4** yields

$$\lambda A(\mathbf{q}; \varepsilon) = \int d\mathbf{u} K(\mathbf{q} - \varepsilon\mathbf{u}/2, \mathbf{u})A(\mathbf{q} - \varepsilon\mathbf{u}; \varepsilon) \times \exp[i\{\Phi(\mathbf{q} - \varepsilon\mathbf{u}) - \Phi(\mathbf{q})\}/\varepsilon]. \qquad [9]$$

Under the limit $\varepsilon \downarrow 0$, q fixed, Eq. **9** becomes

$$\int d\mathbf{u}\, K(\mathbf{q}, \mathbf{u})\exp\left[-i\mathbf{u} \cdot \frac{\partial\Phi}{\partial\mathbf{q}}(\mathbf{q})\right] = \lambda. \qquad [10]$$

The structure of Eq. **10** becomes more transparent with the definition

$$\tilde{K}(\mathbf{q}, \mathbf{p}) = \int d\mathbf{u}\, K(\mathbf{q}, \mathbf{u})\exp[-i\mathbf{p} \cdot \mathbf{u}] \qquad [11]$$

introduced by Wigner (8) in another context, which we term the Wigner transform. Eq. **10** then becomes the first-order partial differential equation,

$$\tilde{K}(\mathbf{q}, \mathbf{p}) = \lambda, \mathbf{p} = \frac{\partial\Phi}{\partial\mathbf{q}}. \qquad [12]$$

If K is hermitian, then $\tilde{K}$ is real for real $\mathbf{p}$ and $\mathbf{q}$.

On taking the expansion of Eq. **9** to $0(\varepsilon)$ we find

$$\int d\mathbf{u}\left[K\mathbf{u} \cdot \frac{\partial A}{\partial\mathbf{q}} + \frac{1}{2}A\mathbf{u} \cdot \frac{\partial K}{\partial\mathbf{q}} - \frac{i}{2}KAu_mu_n\frac{\partial^2\Phi}{\partial q_m\partial q_n}\right] \times \exp[-i\mathbf{u} \cdot \mathbf{p}] = 0. \qquad [13]$$

In Eq. 13 A represents the first term of the development in ε. Since higher orders will not be pursued a notational change is not deemed necessary. As a consequence of Eq. 11, Eq. 13 may be written in the form of the continuity equation,

$$\frac{\partial}{\partial \mathbf{q}} \cdot (A^2 \tilde{K}_{\mathbf{p}}) = 0, \qquad [14]$$

in which $\tilde{K}_{\mathbf{p}} = \partial/\partial \mathbf{p}\ \tilde{K}(\mathbf{q}, \mathbf{p})$ plays the role of a streaming velocity.

It is of interest to note that in spite of the nonlocal character of the basic equation (1), the development results in local equations (12 and 14). Thus, asymptotically the Wigner transform (11) produces a local equation in $(\mathbf{q}, \mathbf{p})$ space irrespective of whether the original formulation (1) in $(\mathbf{x}, \mathbf{y})$ space is local or not.

Integration of Eq. 12 follows standard lines (9). Along characteristic curves

$$\frac{d\mathbf{q}}{dt} = \frac{\partial \tilde{K}}{\partial \mathbf{p}}, \qquad \frac{d\mathbf{p}}{dt} = -\frac{\partial \tilde{K}}{\partial \mathbf{q}}. \qquad [15]$$

The phase changes according to

$$\frac{d\Phi}{dt} = \mathbf{p} \cdot \frac{d\mathbf{q}}{dt}. \qquad [16]$$

The time t is simply the natural coordinate along the trajectories (Eq. 15). Viewed as a dynamical system Eq. 15 has the hamiltonian $\tilde{K}$ as an invariant, $\tilde{K} = \lambda$ (Eq. 12). Unlike a true dynamical system, neither the time nor the dependence of $\mathbf{q}$ on it is of essential importance in the solution of the original problem.

Features of the eigenvalue problem follow from consideration of the hamiltonian system (Eq. 15). A clear dichotomy is based on the question of whether Eq. 15 is completely integrable (10, 11). In the event that it is, then the orbit of the dynamical system (Eq. 15) is restricted to an N-torus, and the system (Eq. 15) possesses N invariants—(the actions)

$$J_k = \oint_{\gamma_k} \mathbf{p}\, d\mathbf{q}; \qquad k = 1, \ldots, N, \qquad [17]$$

where the curves γ_k refer to the N independent irreducible circuits of the torus. This is the case treated by Keller (6) in his classic paper. Our derivation shows that his treatment applies to the more general case developed above.

From Eq. 14 it is seen that the amplitude, A, diverges when bundles of characteristics constrict so that the cross-section loses dimensions or when the flux velocity vanishes. The loci of such points form the caustics of the integrated equations, and the solution undergoes a change in phase at such boundaries. The generic result is that a phase change of $\pi/2$ results for each dimension lost or for each momemtum that changes signature (6). As a consequence, Eq. 7 will yield a single-valued solution only if

$$J_k = 2\pi(\nu_k + \mu_k/4)\varepsilon, \qquad k = 1, \ldots, N, \qquad [18]$$

which is known as the Einstein–Brillouin–Keller formula (11). Both ν_k and μ_k are integers and the latter is referred to as the Maslov index (12). A consequence of this discussion is that operators having the same action integrals have, asymptotically, the same eigenvalues. Under certain circumstances this is exact (13).

In the event that Eq. 15 is not completely integrable the situation is more difficult to treat and the corresponding eigenvalues have been termed the irregular spectrum (14). Although such hamiltonian systems now are better understood from the Kolmogorov–Arnold–Moser theorem (15), the behavior of the irregular spectrum remains unclear and the relevance of the WKB method itself for such situations is not certain (16).

It should not go unnoticed that such well-understood objects as say regular Fredholm operators lead to the rich variety of nonlinear dynamical problems that are widely discussed in the current literature (17).

One-Dimensional Case—An Area Rule (1–3)

In this instance, the dynamics may be avoided since the solutions of Eq. 15 are simply the contours of Eq. 12. A typical contour is sketched in Fig. 1. If we denote the branches by $p_m(q; \lambda)$, then "time" is trivially eliminated from Eq. 16 and we write

$$\frac{d\Phi_m}{dq} = p_m(q; \lambda). \qquad [19]$$

The amplitude equation (14) yields

$$A_m \propto [\tilde{K}_p(p_m(q), q)]^{-1/2}, \qquad [20]$$

which diverges at the four vertical tangents, or turning points, indicated in the figure. In traversing the contour in the sense shown, the phase is found to increment at convex turning points by $\pi/2$ while at concave turning points it decrements by $\pi/2$ (1). For any simple closed loop there are two more convex than concave turning points and we obtain

$$\oint_\gamma p\, dq = \mathcal{A}(\lambda) = 2\pi\left(\nu + \frac{1}{2}\right)\varepsilon, \qquad [21]$$

where ν is an integer and $\mathcal{A}(\lambda)$ refers to the area enclosed by the curve $\tilde{K}(q, p) = \lambda$. (The Maslov index is 2.) We refer to Eq. 21 as the area rule.

A Class of Separable Problems

Consider the class of kernels, invariant under rotation and of the form

$$K(\mathbf{q}, \mathbf{u}) = K(q, u) = K(\varepsilon|\mathbf{x} + \mathbf{y}|/2, |\mathbf{x} - \mathbf{y}|). \qquad [22]$$

Kernels of this type occur in the study of vision, in which case they operate in two dimensions (18). To introduce notation and for later use we briefly consider the eigenvalue problem based on the Laplace operator,

$$\nabla^2 \psi = -k^2 \psi. \qquad [23]$$

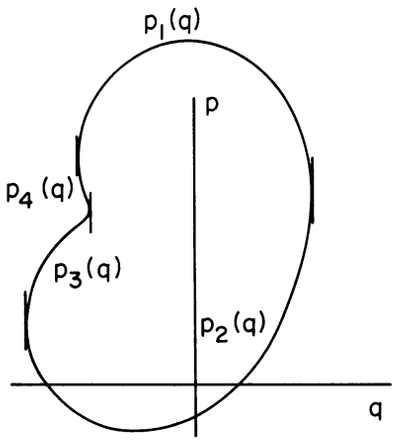

FIG. 1. Typical contour for $\tilde{K}(q, p) = \lambda$. Turning points are indicated by vertical tangents and branches by $p_k(q)$, $k = 1, \ldots, 4$.

In N dimensions,

$$\nabla^2 = \frac{1}{r^{n-1}} \frac{\partial}{\partial r} r^{n-1} \frac{\partial}{\partial r} + \frac{1}{r^2}\mathcal{L}, \quad [24]$$

where $\mathcal{L}$ refers to the angular part of the laplacian. We denote spherical harmonics by $S_{\mathbf{m}(n)}$ so that

$$\mathcal{L}S_{\mathbf{m}(n)} = -n(n + N - 2)S_{\mathbf{m}(n)}. \quad [25]$$

By $\mathbf{m}(n)$ is meant the $N - 1$ indices associated with the "radial" index n. Thus, if we write

$$\psi_n = \mathcal{J}_n(r)S_{\mathbf{m}(n)}, \quad [26]$$

we find

$$\mathcal{J}_n(r) = J_{n-1+N/2}(kr), \quad [27]$$

where J_m refers to the Bessel function of index m.

The spherical symmetry of Eq. **22** implies that its eigenfunctions are products of radial eigenfunctions and spherical harmonics. Therefore, instead of Eq. **7** we write

$$\psi_{\mathbf{m}(n)} = S_{\mathbf{m}(n)}A_n(q; \varepsilon)\exp[i\phi_n(q)/\varepsilon]. \quad [28]$$

If Eq. **28** is introduced into Eq. **4**, then under the limit $\varepsilon \downarrow 0$ we find

$$\tilde{K}(q, p) = \lambda, \quad [29]$$

where

$$p = p(\rho, q) = [\rho^2(q) + \varepsilon^2(n - 1 + N/2)^2/q^2]^{1/2},$$

$$\rho = \frac{\partial\phi(q)}{\partial q}. \quad [30]$$

In terms of the underlying dynamical problem as represented by Eq. **15**, Eq. **30** represents the radial momentum component. It is interesting to note that if Eq. **28** is introduced into the Helmholtz equation (**23**), we get the "exact" value $n(n + N - 2)$ instead of the above asymptotic value $[n + (N/2) - 1]^2 = n(n + N - 2) + [(N/2) - 1]^2$. It should also be noted that for n fixed $\varepsilon \downarrow 0$, the second term of the first argument disappears (see discussion below). This term is retained for n large and Eq. **29**; Eq. **30** represents a uniform approximation.

At the next order we obtain the amplitude equation (**14**), which yields in this case,

$$A \propto \left\{q^{N-1} \frac{\partial}{\partial\rho} \tilde{K}(q, p(\rho, q))\right\}^{-1/2}. \quad [31]$$

For the class of kernels (**22**) the problem is reduced to an equivalent one-dimensional problem as specified by Eqs. **29** and **31**. At this point the procedure depends on the contour plots of Eq. **29** in the $(\rho - q)$ plane and the one-dimensional treatment given above can be referred to (1–3). In particular, the various turning points as determined by the vanishing of $\tilde{K}_\rho$ in Eq. **31** locate the points of attachment for the corresponding branches of Eq. **29**. An important modification is that the origin $q = 0$ is an additional critical point as Eq. **31** indicates. An analysis of this region demonstrates that solutions there take on the behavior of the Bessel functions as in Eq. **27** and that these must be attached to the conventional WKB form of the solution. Further discussion depends on the particular topology of Eq. **29** and particularly on the branch structure that is implied by Eq. **29**. As an illustration we consider the case in which a typical level line of Eq. **29** has the form shown in Fig. 2; the assumption is that $\tilde{K}$ is even in p and that only two branches appear. The form of $\rho = \rho(q)$ then follows from Eq. **30** and the two limits $\varepsilon \downarrow 0$, n fixed and $n = 0(1/\varepsilon)$ and are shown in Figs. 3 and 4, respectively. In the second case since the contour is bounded away from the origin the one-dimensional analysis applies. Thus,

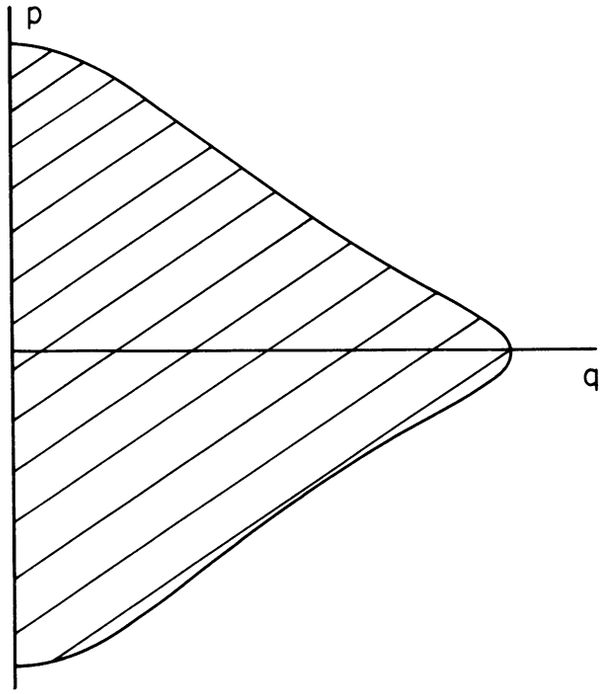

FIG. 2. Typical contour of Eq. **29** when $\tilde{K}$ is even in p and two branches occur.

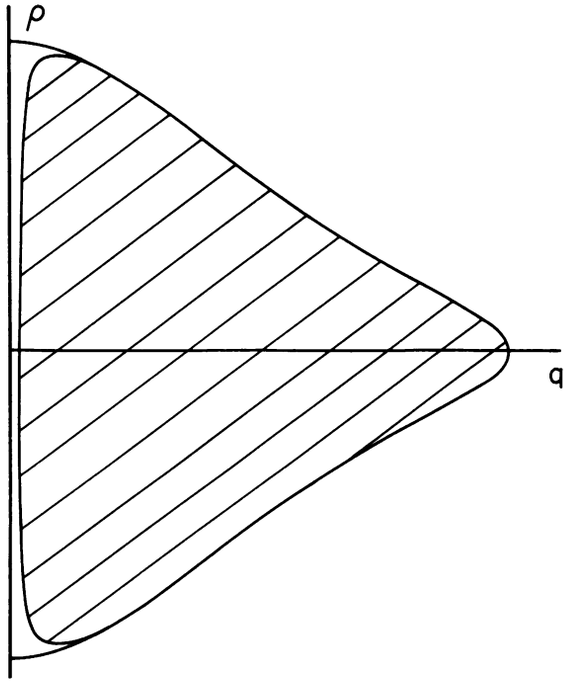

FIG. 3. Inner curve, typical contour of $\rho = \rho(q)$ as determined by Eq. **30**, when $m = 0(1)$; outer curve corresponds to $m = 0$ and is the same as Fig. 2.

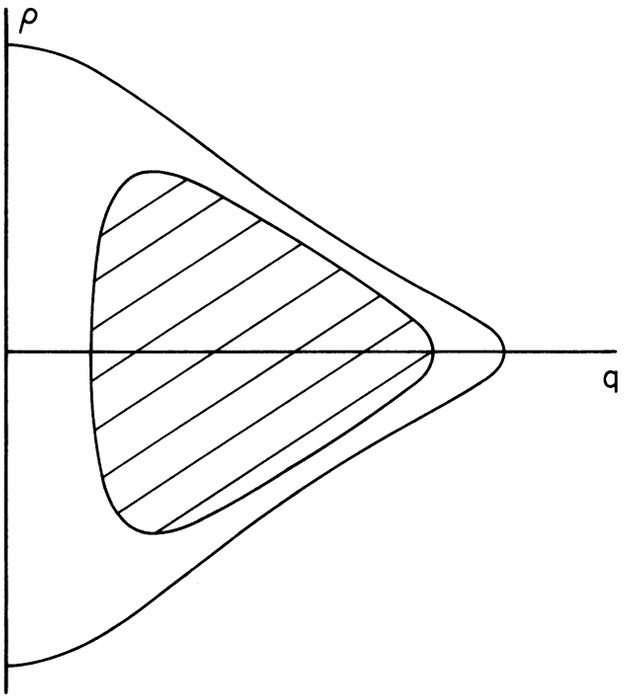

FIG. 4. Inner curve, $m = 0(\varepsilon^{-1})$; outer curve, as in Fig. 3.

the condition that λ be an eigenvalue is the same as Eq. **21**, namely,

$$\oint_\gamma p(q)dq = 2\pi\left(\nu + \frac{1}{2}\right)\varepsilon \qquad [32]$$

(ν an integer), where the area is the hatched portion shown in Fig. 4. On the other hand, the case depicted in Fig. 3 is complicated by the fact that the Bessel function behavior in the neighborhood of the origin overlaps the inner turning point. In this case it may be shown that the condition that λ be an eigenvalue is that

$$\oint_\gamma p(q)dq = 2\pi\left(\nu + m + \frac{1}{2}\right)\varepsilon, \qquad [33]$$

where the area now refers to the hatched portion of Fig. 2. It is an interesting fact that formula **32** may be shown to yield Eq. **33** in the limit $\varepsilon \downarrow 0$, m fixed, and is a uniformly valid condition for λ to be an eigenvalue.

Extension to Systems

Both the general analysis and the particular cases treated above can be directly extended to the case of systems. To briefly indicate the modification we now regard K as a matrix and ψ a vector in Eq. **4**, and thus A in Eq. **7** is a vector while Φ remains a scalar. At lowest order we find

$$(\bar{K}(\mathrm{q}, \mathrm{p}) - \lambda)l = 0 \qquad [34]$$

$$A \propto l. \qquad [35]$$

The eigenvector l is a function of position. The constant λ is forced to be the characteristic value of Eq. **34** through the condition

$$\det\left[\bar{K}\left(\mathrm{q}, \frac{\partial\Phi}{\partial \mathrm{q}}\right) - \lambda\right] = 0, \qquad [36]$$

which in turn determines the phase. The proportionality factor in Eq. **35** is also a function of position that can be determined by proceeding to the next order in the analysis. If this is denoted by α, we then find

$$\alpha = [(l, \bar{K}_p l)]^{-\frac{1}{2}}. \qquad [37]$$

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