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An exact WKB method for 2×2 systems and applications

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1. Basic thoery of an exact WKB method

We study 2×2 systems of first order differential equations

$$\frac{h}{i}\frac{d}{dx}\mathbf{u} = M(x,h)\mathbf{u}, \tag{1}$$

where the unknown function $\mathbf{u}(x,h) = {}^t(u_1(x,h), u_2(x,h))$ is a column vector, $M(x,h)$ is a 2×2 matrix valued function and h is a small parameter. By conjugating the system with the function

$$\exp\left(-\frac{i}{h}\int^x \mathrm{Tr}\, M(t,h)\, dt\right),$$

we can assume M is trace-free:

$$M(x,h) = \begin{pmatrix} a(x,h) & b(x,h) \\ c(x,h) & -a(x,h) \end{pmatrix}. \tag{2}$$

The eigenvalues of M are $\pm i\sqrt{\det M} = \pm iz'$. The zeros of $\det M(x,h)$ are called the *turning points* of the system (1). In this section, we assume

(H0): M is independent of h and $M \in \mathcal{H}(\Omega, GL(2,\mathbb{C}))$, i.e. the elements $a(x,h)$, $b(x,h)$ and $c(x,h)$ are analytic in a complex domain Ω and there is no turning point there.

1.1. **Formal construction.** We define the phase function $z(x,h)$ by

$$z(x;\alpha) = \int_\alpha^x \sqrt{\det M(t)}\, dt, \tag{3}$$

for a fixed point α, and we look for solutions of the form

$$\mathbf{u}_\pm(x,h) = e^{\pm z(x,h)/h} Q(x) \begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix}^{\frac{1\pm 1}{2}} \mathbf{w}^\pm(x,h), \tag{4}$$

$$\mathbf{w}^\pm(x,h) = \sum_{n=0}^\infty \mathbf{w}_n^\pm(x,h), \quad \mathbf{w}_0^\pm(x,h) \equiv \begin{pmatrix} 1 \\ 0 \end{pmatrix}, \tag{5}$$

where the sums are absolutely convergent in a neighborhood of a fixed point $x_0 \in \Omega$, i.e. $u_\pm$ are exact solutions and, moreover, they give asymptotic expansions of $u_\pm$ as $h \to 0$ in a subdomain $\Omega^\pm$, which will be defined later.

Lemma 1.1. *There exists $Q(x) \in \mathcal{H}(\Omega, GL(2,\mathbb{C}))$ such that the followings hold:*

$$Q^{-1}MQ = \begin{pmatrix} iz' & 0 \\ 0 & -iz' \end{pmatrix}, \tag{6}$$

$$Q^{-1}Q' = -\begin{pmatrix} 0 & c_+(x) \\ c_-(x) & 0 \end{pmatrix} \quad \text{for some} \quad c_\pm(x) \in \mathcal{H}(\Omega, \mathbb{C}), \tag{7}$$

where $'$ stands for the derivative with respect to x. Such matrix $Q(x)$ is unique up to multiplication from the right by a diagonal constant matrix.

Proof. Since Ω is turning point free, the matrix M is diagonalizable in Ω by a regular analytic matrix $P = P(x,h)$:

$$P^{-1}MP = \begin{pmatrix} iz' & 0 \\ 0 & -iz' \end{pmatrix}.$$

Put

$$P^{-1}P' = C(x) = \begin{pmatrix} c_{11}(x) & c_{12}(x) \\ c_{21}(x) & c_{22}(x) \end{pmatrix}. \tag{8}$$

Then $Q(x)$ and $c_\pm(x)$ are given by

$$Q(x) = P(x)E(x), \quad E(x) = \begin{pmatrix} \exp(-\int c_{11}(x)dx) & 0 \\ 0 & \exp(-\int c_{22}(x)dx) \end{pmatrix},$$

$$c_+(x) = -c_{12}(x)\exp\left\{\int (c_{11}(x) - c_{22}(x))dx\right\},$$

$$c_-(x) = -c_{21}(x)\exp\left\{\int (c_{22}(x) - c_{11}(x))dx\right\}.$$

□

Remark 1.2. *As a consequence from (7),* $\det Q(x)$ *is independent of x. Indeed, (7) implies*

$$\frac{d}{dx}(\det Q) = -\mathrm{Tr}\begin{pmatrix} 0 & c_+(x) \\ c_-(x) & 0 \end{pmatrix}\det Q = 0.$$

Lemma 1.3. *If the matrix M is anti-diagonal*

$$M(x) = \begin{pmatrix} 0 & g_+(x) \\ -g_-(x) & 0 \end{pmatrix}, \tag{9}$$

the matrix $Q(x)$ and the functions $c^\pm(x)$ are given by

$$Q(x) = \begin{pmatrix} H(x)^{-1} & H(x)^{-1} \\ iH(x) & -iH(x) \end{pmatrix}, \quad c^+(x) = c^-(x) = \frac{H'(x)}{H(x)},$$

where

$$H(x) = \left(\frac{g_-(x)}{g_+(x)}\right)^{1/4}.$$

The functions $\mathbf{w}^{\pm}$ in (4) satisfy

$$\frac{d\mathbf{w}^{\pm}}{dx} + \begin{pmatrix} 0 & 0 \\ 0 & \pm 2z'/h \end{pmatrix} \mathbf{w}^{\pm} = \begin{pmatrix} 0 & c^{\mp} \\ c^{\pm} & 0 \end{pmatrix} \mathbf{w}^{\pm}, \tag{10}$$

or regarding $w^{\pm}$ as functions of z,

$$\frac{d\mathbf{w}^{\pm}}{dz} + \begin{pmatrix} 0 & 0 \\ 0 & \pm 2/h \end{pmatrix} \mathbf{w}^{\pm} = \frac{1}{z'} \begin{pmatrix} 0 & c^{+} \\ c^{-} & 0 \end{pmatrix} \mathbf{w}^{\pm}, \tag{11}$$

where z' and $c^{\pm}$ are also regarded as functions of z in the second equations.

We can formally construct solutions of these systems in the form (5) with

$$\mathbf{w}_n^{\pm} = \begin{pmatrix} w_{2n}^{\pm} \\ w_{2n-1}^{\pm} \end{pmatrix}, \tag{12}$$

by determining inductively the functions $w_n(z,h)$ by

$$w_{-1}^{\pm} \equiv 0, \quad w_0^{\pm} \equiv 1, \tag{13}$$

and for $n \geq 1$,

$$\begin{cases} \frac{d}{dx} w_{2n}^{\pm} & = c^{\mp}\, w_{2n-1}^{\pm}, \\ \left(\frac{d}{dx} \pm \frac{2}{h} z'(x)\right) w_{2n-1}^{\pm} & = c^{\pm}\, w_{2n-2}^{\pm}, \end{cases} \tag{14}$$

or equivalently,

$$\begin{cases} \frac{d}{dz} w_{2n}^{\pm} & = \frac{c^{\mp}}{z'}\, w_{2n-1}^{\pm}, \\ \left(\frac{d}{dz} \pm \frac{2}{h}\right) w_{2n-1}^{\pm} & = \frac{c^{\pm}}{z'}\, w_{2n-2}^{\pm}. \end{cases} \tag{15}$$

The recurrence equations (14) with initial conditions

$$w_n^{\pm}|_{x=x_0} = 0 \quad (n \geq 1) \tag{16}$$

uniquely determine the sequence of scalar functions $\{w_n^{\pm}(x,h;x_0)\}_{n=-1}^{\infty}$ and the sequence of vector functions $\{\mathbf{w}_n^{\pm}(x,h;x_0)\}_{n=0}^{\infty}$. Let us write

$$w_{\text{even}}^{\pm}(x,h;x_0) = \sum w_{2n}^{\pm}(x,h;x_0), \quad w_{\text{odd}}^{\pm}(x,h;x_0) = \sum w_{2n-1}^{\pm}(x,h;x_0),$$

Thus we have constructed formal solutions (4), which we write from now on $\mathbf{u}_{\pm}(x,h;\alpha,x_0)$, depending on a base point α for the phase and a base point x_0 for the amplitude.

Theorem 1.4. *The exact WKB solutions $\mathbf{u}_{\pm}(x,h;\alpha,x_0)$ have the following three properties:*

(i) *The formal series (5) are absolutely convergent in a neighborhood of x_0.*

(ii) *Let $\Omega_{\pm}$ be the set of $x \in \Omega$ such that there exists a path from x_0 to x in Ω along which $\pm\mathrm{Re}z(x)$ increases strictly. Then we have for each $N \in \mathbb{N}$*

$$\mathbf{w}^{\pm} - \sum_{n=0}^{N-1} \mathbf{w}_n^{\pm} = O(h^N),$$

uniformly in any compact subset of $\Omega_{\pm}$.

(iii) *The Wronskian of any two exact WKB solutions of different sign with different base points of amplitude are given by*

$$\mathcal{W}(\mathbf{u}^+(x,h;\alpha,x_0),\mathbf{u}^-(x,h;\alpha,x_1)) = -\det Q\ w^+_{\text{even}}(x_1,h;x_0), \tag{17}$$

where $\mathcal{W}(\mathbf{f},\mathbf{g})$ *is by definition the determinant of the matrix* $(\mathbf{f},\mathbf{g})$.

Proof. The proof of the first and the second parts are just the same as in [1], [2], [3], and we only check the third part.

From (4), we immediately have

$$\begin{aligned}
&\mathcal{W}(\mathbf{u}^+(x,h;\alpha,x_0),\mathbf{u}^-(x,h;\alpha,x_1))\\
&= \det Q\ \mathcal{W}\left(\begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix}\mathbf{w}^+(z,x_0),\mathbf{w}^-(z,x_1)\right)\\
&= \det Q\ (w^+_{\text{odd}}(x,h;x_0)w^-_{\text{odd}}(x,h;x_1) - w^+_{\text{even}}(x,h;x_0)w^-_{\text{even}}(x,h;x_1)).
\end{aligned}$$

This must be independent of x since the matrix M is trace free. Hence we can replace x in the right hand side by a particular point, say $x = x_1$. Then taking (13) and (16) into accont, we get (17). □

This theorem enables us not only to construct exact solutions in each turning point free complex domain but also to connect these solutions using the Wronskian formula (17). In particular, if the base points of these WKB solutions are connected by a *canonical* curve along which the real part of the phase increases in the *good* direction, we can know the asymptotic behavior of the Wronskian, i.e. the connection coefficients. Thus we can *generically* know the global asymptotic behavior of solutions.

2. Applications

In this setion, we expose some typical problems of mathematical physics to which our method of the previous section can be applied.

2.1. **1-d Schrödinger equation.** 1-d Schrödinger equation

$$-h^2\frac{d^2u}{dx^2} + V(x)u = Eu$$

is reduced by putting ${}^t\mathbf{u} = (u, -ih\frac{du}{dx})$ to the form (1) with

$$M(x) = \begin{pmatrix} 0 & 1 \\ -(V(x)-E) & 0 \end{pmatrix},$$

which is of the form (9). Hence, by Lemma 1.3, the first component of the vector valued solution (4) is:

$$u_\pm(x,h) = (V(x)-E)^{-1/4}e^{\pm\int^x (V-E)^{1/2}dx/h}\left(w^\pm_{\text{even}}(x,h) + w^\pm_{\text{odd}}(x,h)\right),$$

which are the exact WKB solutions introduced in [3]. This method was applied to the double-well eignevalue asymptotics ([3]) and semiclassical 1-d scattering problems ([6], [2] etc.)

2.2. **2-level adiabatic transition.** If $x = t$ is a time variable, the equation (1) can be considered as a time-dependent 2-level Schrödinger equation with Hamiltonian $-M(t,h)$. The small parameter h is the semiclassical or adiabatic parameter. M is often supposed to be real symmetric

$$M(t,h) = \begin{pmatrix} a(t,h) & b(t,h) \\ b(t,h) & -a(t,h) \end{pmatrix}.$$

By the change of the unknown

$$\mathbf{u} = \frac{1}{\sqrt{2}} \begin{pmatrix} 1 & i \\ i & 1 \end{pmatrix} \mathbf{v}$$

(1) can also be reduced to the form (9):

$$\frac{h}{i}\frac{d}{dx}\mathbf{v} = \begin{pmatrix} 0 & ia+b \\ -(ia-b) & 0 \end{pmatrix} \mathbf{v}.$$

In this case, one has

$$z(x,h) = i\int^x (a^2+b^2)^{1/2}dx, \quad H = \left(\frac{a+ib}{a-ib}\right)^{1/4}.$$

2.3. **Langer modification.** 3-d Schrödinger equation with radially symmetric potential is reduced to the 1-d equation with respect to the radial variable r:

$$-h^2\frac{d^2u}{dr^2} + V(r)u + \frac{h^2 l(l+1)}{r^2}u = Eu. \tag{18}$$

For this equation, $r = 0$ is a regular singular point with Fuchsian indices $l+1, -l$. The principal terms of the usual WKB solutions (so called Liouville Green functions) are

$$(V(r) - E + \frac{h^2 l(l+1)}{r^2})^{-1/4} \exp\left\{\pm\frac{1}{h}\int^r (V(r) - E + \frac{h^2 l(l+1)}{r^2})^{1/2}dr\right\},$$

and they behave asymptotically like $r^{\pm\sqrt{l(l+1)}+1/2}$ as $r \to 0$ (while $h > 0$ is fixed). The exponents apparently differ from the Fuchsian indices, and this means that the WKB approximations in this direction are not uniformly accurate when r is small. This change of exponents from $l(l+1)$ to $(l+\frac{1}{2})^2$ is often called *Langer modification*, and since his own work [5], many different approaches have been tried to know the monodromy around a regular singular point (see for example [2], [4] for very recent references).

The following reduction to a system is also one of such approaches. Put

$${}^t\mathbf{u} = \left(r^{-1/2}u, \frac{h}{i}r\frac{d}{dr}r^{-1/2}u\right).$$

Then (18) is reduced to

$$\frac{h}{i}\frac{d}{dr}\mathbf{u} = \frac{1}{r}\begin{pmatrix} 0 & 1 \\ -r^2(V(r)-E) - h^2(l+\frac{1}{2})^2 & 0 \end{pmatrix}\mathbf{u}. \tag{19}$$

$r = 0$ is a regular singular point also for this system and the Fuchsian indices are $\pm(l + 1/2)$. On the other hand, the principal terms of the exact WKB solutions constructed for (19) in our way are

$$\mathbf{u}_\pm(r,h) \sim e^{\pm z(r,h)/h} \begin{pmatrix} H(r,h)^{-1} \\ \mp iH(r,h) \end{pmatrix}, \tag{20}$$

where

$$z(r,h) = \int^r \sqrt{r^2(V(r)-E) + h^2(l+1/2)^2}\,\frac{dr}{r},$$

$$H(r,h) = \left(r^2(V(r)-E) + h^2(l+1/2)^2\right)^{1/4}.$$

Since $z(r,h) \sim (l+\frac{1}{2})\log r$ and $H(r,h) \sim h^{1/2}(l+\frac{1}{2})^{1/2}$ as $r \to 0$ while $h > 0$ is fixed, the right hand side of (20) behaves like constant times $r^{\pm(l+1/2)}$, which coincides with the Fuchsian indices.

As a matter of fact, it can be shown that the subdominant solution at the origin to (19) corresponding to the index $l+\frac{1}{2}$ (which corresponding the regular solution to (18)) is colinear to the exact WKB solution $\mathbf{u}_+(r,h;\alpha,0)$ whose phase $z(r,h)$ is determined so that its real part is decreasing as r tends to 0 and whose base point for the symbol is taken at the origin. Note that, in this case, the recurence relations (14) becomes of regular singular type equations at $r=0$ with 0 initial data there.

2.4. **A model of conical intersection.** In [1], the semiclassical distribution of resonances of the following model of 2-d 2-level Schrödinger equation is studied:

$$-h^2\Delta\mathbf{u} + \begin{pmatrix} x_1 & x_2 \\ x_2 & -x_1 \end{pmatrix}\mathbf{u} = E\mathbf{u}$$

This second order equation is reduced to a first order one by h-Fourier transform:

$$\hat{\mathbf{u}}(\xi) = \frac{1}{2\pi h}\int_{\mathbb{R}^2} e^{-ix\cdot\xi/h}\mathbf{u}(x)dx.$$

Using the polar coordinate $\xi = r(\cos\theta, \sin\theta)$ and developing $\hat{\mathbf{u}}(\xi)$ in Fourier series after some change of the unknown function

$$\hat{\mathbf{u}}(\xi) = r^{1/2}\begin{pmatrix} \cos\frac{\theta}{2} & -\sin\frac{\theta}{2} \\ \sin\frac{\theta}{2} & \cos\frac{\theta}{2} \end{pmatrix} \sum_{l=-\infty}^{\infty} e^{i(l+1/2)\pi\theta/h}\mathbf{v}_l(r),$$

we get the following reduced equations for $\mathbf{v}_l(r)$:

$$\frac{h}{i}\frac{d}{dr}\mathbf{v}_l = \begin{pmatrix} r^2 - E & (l+\frac{1}{2})h/r \\ -(l+\frac{1}{2})h/r & E - r^2 \end{pmatrix}\mathbf{v}_l. \tag{21}$$

This equation has a regular singular point at $r = 0$ and the Fuchsian indices are $\pm(l + 1/2)$.

Conjugated with a constant matrix $\frac{1}{\sqrt{2}}\begin{pmatrix} 1 & -1 \\ 1 & 1 \end{pmatrix}$, this equation becomes again of the form (9), and we can construct exact WKB solutions as in the previous section. Their principal terms are given by (20) where

$$z(r,h)=\int^{r}\sqrt{(l+1/2)^2h^2-r^2(E-r^2)^2}\,\frac{dr}{r},$$

$$H(r,h)=\left(\frac{(l+1/2)h+Er-r^3}{(l+1/2)h-Er+r^3}\right)^{1/4}.$$

In this case also, the physically interesting solution to (21) is colinear to the exact WKB solution constructed with the phase whose real part decreases as $r\to 0$ (see [1]).

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