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Semi-classical Asymptotics for Local Spectral Densities and Time Delay Problems in Scattering Processes

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We study the semi-classical asymptotics for local spectral densities of Schrödinger operators $-\frac{1}{2}h^2\Delta + V$ and apply the obtained result to the time delay problem in potential scattering theory. It is shown that for a class of central potentials, the time delay in quantum mechanics converges to the corresponding one in classical mechanics in the semi-classical limit in a non-trapping energy region. However, such a convergence is not expected in a trapping energy region.

0. INTRODUCTION

In the present paper we study the semi-classical asymptotics for local spectral densities of Schrödinger operators $H(h) = -\frac{1}{2}h^2\Delta + V$, $0 < h \leqslant 1$, in the n-dimensional space R^n_x, $n \geqslant 2$, and apply the obtained results to time delay problems in scattering processes.

We begin by defining the local spectral densities above, which are essentially energy derivatives of spectral functions. We first make the following assumptions on the potential $V(x)$:

Assumption $(V)_\rho$. $V(x)$ is a real C^∞-smooth function and satisfies

$$|\partial_x^\alpha V(x)| \leqslant C_\alpha \langle x \rangle^{-\rho - |\alpha|}$$

for some $\rho > 0$, where $\langle x \rangle = (1 + |x|^2)^{1/2}$.

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We denote by $E(\lambda; H(h))$ the spectral resolution associated with $H(h)$,

$$H(h)=\int_{-\infty}^{\infty} \lambda \, dE(\lambda; H(h)),$$

and by $R(z; H(h))$, $\operatorname{Im} z \neq 0$, the resolvent of $H(h)$, $R(z; H(h)) = (H(h)-z)^{-1}$. Under the assumption $(V)_\rho$ with $\rho > (n+1)/2$, the principle of limiting absorption yields the well-known relation

$$\begin{aligned} E'(\lambda; H(h)) &= (d/d\lambda) E(\lambda; H(h)) \\ &= (2\pi i)^{-1} (R(\lambda + i0; H(h)) - R(\lambda - i0; H(h))) \end{aligned}$$

for $\lambda > 0$ and also the integral kernel $e'(x, y; \lambda, h)$, $\lambda > 0$, of $E'(\lambda; H(h))$ is represented in terms of the generalized eigenfunctions of $H(h)$.

Let B be a bounded open set in R^n_x and let I be a bounded interval in $(0, \infty)$. Denote by χ_B and χ_I the characteristic functions of B and I, respectively. We define $\sigma_h(B \times I)$ by

$$\sigma_h(B \times I) = (2\pi h)^n \operatorname{Tr}(\chi_B \chi_I(H(h)) \chi_B).$$

Then we have

$$d\sigma_h(x, \lambda) = (2\pi h)^n e'(x, x; \lambda, h) \, dx \, d\lambda.$$

According to Lavine [16], we shall call $\sigma_h(x, \lambda)$, $(x, \lambda) \in R^n_x \times (0, \infty)$, the local spectral density for $H(h)$. The corresponding quantity in classical mechanics is defined by

$$\sigma_0(B \times I) = \operatorname{vol}(\{x, \xi): \tfrac{1}{2} |\xi|^2 + V(x) \in I, x \in B\})$$

and hence

$$d\sigma_0(x, \lambda) = n\omega_n((2\lambda - 2V(x))_+)^{n/2-1} \, dx \, d\lambda,$$

where ω_n denotes the volume of the n-dimensional unit ball and $f_+(x) = \max(0, f(x))$. We know [16, 21] that

$$(2\pi h)^n e'(x, x; \lambda, h) \to n\omega_n((2\lambda - 2V(x))_+)^{n/2-1}$$

as $h \to 0$ in the distribution sense (i.e., in $D'(R^n_x \times (0, \infty))$). In the first half of the present paper, we will show that the above convergence holds in $D'(R^n_x)$, if energy λ is restricted to a certain energy region (non-trapping energy region).

We shall formulate the above result more precisely. In addition to $(V)_\rho$ with $\rho > (n+1)/2$, we assume that energy $\lambda > 0$ under consideration is non-trapping in the following sense.

Non-trapping Condition. Let $\{x(t; y, \eta), \xi(t; y, \eta)\}$ be the solution to the Hamilton system $\dot{x} = \xi$, $\dot{\xi} = -\nabla V$ with initial state (y, η). We say that energy $\lambda > 0$ is non-trapping, if for any $R \gg 1$ large enough, there exists $T = T(R)$ such that $|x(t; y, \eta)| > R$ for $|t| > T$ when $|y| < R$ and $\lambda = \frac{1}{2}|\eta|^2 + V(y)$.

Under the above assumptions, the main theorem can be formulated as

THEOREM 0.1. *Assume $(V)_\rho$ with $\rho > (n+1)/2$ and that $\lambda > 0$ is non-trapping. Let $W(x) \in C^\infty(R^n_x)$ be a function such that for $\nu > n$*

$$|\partial_x^\alpha W(x)| \leqslant C_\alpha \langle x \rangle^{-\nu - |\alpha|}.$$

Then

$$(2\pi h)^n \int_{R^n} W(x) e'(x, x; \lambda, h)\, dx \sim \sum_{j=0}^{\infty} F_j(\lambda) h^j,$$

as $h \to 0$, where the leading term $F_0(\lambda)$ is given by

$$F_0(\lambda) = n\omega_n \int_{R^n} W(x)((2\lambda - 2V(x))_+)^{n/2-1}\, dx.$$

We here make a comment on the pointwise asymptotic expansion in h for $e'(x, x; \lambda, h)$. In [17, 22], the problems on the short-wave (or high-energy) asymptotics for local spectral densities have been studied for second-order elliptic operators with compactly supported perturbed coefficients, and under the non-trapping condition, pointwise expansion formulas have been obtained when x ranges over a compact region. These results will apply to our semi-classical asymptotic problems, if λ is non-trapping and if x is restricted to a compact region, and such formulas will be represented by making use of the Arnold–Keller–Maslov index for the classical trajectories starting from x and coming back to x with energy λ, if such trajectories exist. However, our interest here lies in the global expansion rather than in the local expansion. It seems to be not easy to prove even the uniform bound for $e'(x, x; \lambda, h)$ such as $e'(x, x; \lambda, h) = O(h^{-n})$ uniformly in x. One of the difficulties comes from the fact that the generalized eigenfunction of $H(h)$ itself is not expected to be bounded uniformly in h, because the scattering amplitude $f(\omega \to \theta; \lambda, h)$ for the incoming direction ω has a strong peak in a neighborhood of ω.

The second half is devoted to the application of the above theorem to the time delay problems in scattering processes. We define the (average) time delay in quantum mechanics by the λ-derivatives of spectral shift functions (total scattering phases) in the Birman–Krein trace formula and show that in the semi-classical limit $h \to 0$, this quantity converges to the corresponding one in classical mechanics for a class of central potentials, if λ is in a non-trapping energy region. On the other hand, if λ is in a trapping energy region, this quantity is not expected to converge to the classical one.

1. Spectral Representation

We write $H_0(h) = -\frac{1}{2}h^2\Delta$ and denote by $E(\lambda; H_0(h))$ the spectral resolution associated with $H_0(h)$. We further denote by $\phi_0(x, \lambda, \omega; h)$, $(\lambda, \omega) \in (0, \infty) \times S^{n-1}$, the generalized eigenfunction of $H_0(h)$,

$$\phi_0(x, \lambda, \omega; h) = \exp(ih^{-1}\sqrt{2\lambda}\,\langle x, \omega \rangle),$$

where S^{n-1} denotes the $(n-1)$-dimensional unit sphere and $\langle\,,\rangle$ is the scalar product in R^n. We define $\psi_0(x, \lambda, \omega; h)$ by $\psi_0 = c_0(\lambda, h)\,\phi_0$ with the normalized constant

$$c_0(\lambda, h) = (2\pi h)^{-n/2}\,(2\lambda)^{(n-2)/4}.$$

Then the unitary operator $F_0(h)$: $L^2(R^n_x) \to L^2((0, \infty); L^2(S^{n-1}))$ defined by

$$(F_0(h)\,f)(\lambda, \omega) = \int_{R^n} \bar{\psi}_0(x, \lambda, \omega; h)\,f(x)\,dx \tag{1.1}$$

gives the spectral representation for $H_0(h)$ in the sense that $H_0(h)$ is transformed into the multiplication by λ in the space $L^2((0, \infty); L^2(S^{n-1}))$.

We now assume $(V)_\rho$ with $\rho > (n+1)/2$. Then, according to the principle of limiting absorption, the generalized eigenfunction $\phi_\pm(x, \lambda, \omega; h)$ of $H(h)$ is given by

$$\phi_\pm = \phi_0 - R(\lambda \pm i0; H(h))\,V\phi_0.$$

We define $\psi_\pm(x, \lambda, \omega; h)$ by $\psi_\pm = c_0(\lambda, h)\phi_\pm$ with the same normalized constant $c_0(\lambda, h)$ as above. We denote by L^2_{ac} the absolutely continuous subspace of $H(h)$. Then we can define the unitary operators $F_\pm(h)$: $L^2_{ac} \to L^2((0, \infty); L^2(S^{n-1}))$ by

$$(F_\pm(h)f)(\lambda, \omega) = \int_{R^n} \bar{\psi}_\pm(x, \lambda, \omega; h)f(x)\,dx$$

and $F_\pm(h)$ give the spectral representation for $H(h)$ restricted to L^2_{ac} in the same sense as for $H_0(h)$. Therefore, the integral kernel $e'(x, y; \lambda, h)$, $\lambda > 0$, of $E'(\lambda; H(h))$ is represented as

$$e'(x, y; \lambda, h) = \int_{S^{n-1}} \psi_\pm(x, \lambda, \omega; h)\,\bar{\psi}_\pm(y, \lambda, \omega; h)\,d\omega. \tag{1.3}$$

2. Weak Asymptotics

In what follows, we write $p(x, \xi) = \frac{1}{2}|\xi|^2 + V(x)$ and use the abbreviation; integrations with no domains attached are taken over the whole space. In this section we first show without assuming the non-trapping condition that the quantity under consideration

$$\rho_W(\lambda; h) = (2\pi h)^n \int W(x) e'(x, x; \lambda, h)\, dx, \qquad \lambda > 0,$$

has an asymptotic expansion in h in the weak sense (i.e., in the distribution sense).

The next proposition follows from [9] and is proved in exactly the same way as there.

Proposition 2.1. *Assume $(V)_\rho$ with $\rho > 0$. Let $f \in C_0^\infty(R^1)$. Then there exists a formal series $a_f = \sum_{j=0}^\infty a_{f,j}(x, \xi) h^j$ such that*

$$\left\| f(H(h)) - \sum_{j=0}^{N-1} a_{f,j}(x, hD_x) h^j \right\|_{\mathrm{tr}} = O(h^{N-n})$$

for any $N > n$, where $\| \ \|_{\mathrm{tr}}$ denotes the trace norm and the symbols $a_{f,j}(x, \xi)$ take the forms

$$a_{f,0}(x, \xi) = f(p(x, \xi)),$$

$$a_{f,j}(x, \xi) = \sum_{k=3}^{2j+1} p_{jk}(x, \xi) f^{(k)}(p(x, \xi)), \qquad j \geq 1,$$

with a family of universal polynomials $p_{jk}(x, \xi)$ of $\partial_x^\alpha \partial_\xi^\beta p$, $|\alpha| + |\beta| \geq 1$.

As an immediate consequence of the above proposition, we obtain the following

Theorem 2.1. *Assume $(V)_\rho$ with $\rho > (n+1)/2$. Let $W(x)$ be as in Theorem 0.1. Fix an open interval $I \subset (0, \infty)$ such that $p(x, \xi)$ has no critical values in I. Then*

$$\int_0^\infty f(\lambda) \rho_W(\lambda; h)\, d\lambda \sim \sum_{j=0}^\infty \left[\int_0^\infty f(\lambda) F_j(\lambda)\, d\lambda \right] h^j, \qquad h \to 0,$$

for any $f \in C_0^\infty(I)$, *where*

$$F_0 = (d/d\lambda) \iint_{p(x,\xi) < \lambda} W(x)\, dx\, d\xi = n\omega_n \int W(x)((2\lambda - 2V(x))_+)^{n/2-1}\, dx,$$

$$F_j = \sum_{k=3}^{2j+1} (-1)^k (d/d\lambda)^{k+1} \left[\iint_{p(x,\xi) < \lambda} W(x)\, p_{jk}(x, \xi)\, dx\, d\xi \right], \qquad j \geq 1,$$

for $\lambda \in I$, p_{jk} *being as in Proposition* 2.1.

If there are no critical values of $p(x, \xi)$ in a fixed open interval $I \subset (0, \infty)$, it then follows from Theorem 2.1 that $\rho_W(\lambda; h)$ converges to $F_0(\lambda)$ as $h \to 0$ in $D'(I)$. We should note that this result is obtained without assuming that $\lambda \in I$ is non-trapping.

3. Strong Asymptotics

In this section, we prove Theorem 0.1. As a result, we obtain that $\rho_W(\lambda; h)$ converges to $F_0(\lambda)$ as $h \to 0$ in the strong (usual) sense, if λ is restricted to a non-trapping energy region.

Proof of Theorem 0.1. By Theorem 2.1, we have only to prove that $\rho_W(\lambda; h)$ has an asymptotic expansion in h in the strong sense. We prove it through several steps.

(1) We first fix an open interval $I_0 = (\lambda - \varepsilon, \lambda + \varepsilon)$ $(\subset (0, \infty))$ for $\varepsilon > 0$ small enough. We may assume that $\mu \in I_0$ is non-trapping. We now take $g \in C_0^\infty(I_0)$ with $g\,|_{\mu = \lambda} = 1$, and define

$$\rho(\mu; h) = g(\mu) \int W(x) e'(x, x; \mu; h)\, dx.$$

We further define

$$G(t; h) = \exp(-ih^{-1} tH(h))\, g(H(h)), \qquad -\infty < t < \infty.$$

Then we have

$$\mathrm{Tr}(G(t; h)\, W) = \int \exp(-ih^{-1} t\mu)\, \rho(\mu; h)\, d\mu$$

and hence the inverse Fourier transform yields

$$\rho(\mu; h) = (2\pi h)^{-1} \int \exp(ih^{-1} \mu t)\, \mathrm{Tr}(G(t; h)\, W)\, dt.$$

However, we have no nice information on the behavior as $|t| \to \infty$ of $\mathrm{Tr}(G(t; h) W)$. Thus, we consider the cut-off integral. Let $\theta \in C_0^\infty(R^1)$ and define

$$J_\theta(\mu; h) = (2\pi h)^{-1} \int \exp(ih^{-1}\mu t)\theta(t) \,\mathrm{Tr}(G(t; h) W)\, dt.$$

(2) We state some properties of $J_\theta(\lambda; h)$ or $\mathrm{Tr}(G(t; h) W)$ as a series of lemmas. We will prove these lemmas in Section 4.

LEMMA 3.1. *If $\theta \in C_0^\infty((-\tau, \tau))$ for $\tau > 0$ small enough and $\theta = 1$ for t, $|t| < \tau/2$, then $J_\theta(\mu; h)$ has an asymptotic expansion in h,*

$$J_\theta(\mu; h) \sim \sum_{j=0}^{\infty} K_j(\mu) h^{j-n}$$

uniformly in $\mu \in I_0$.

LEMMA 3.2. *Let $\tau > 0$ be as above. Fix $T \gg 1$ arbitrarily. If $\theta \in C_0^\infty((\tau/2, T))$ or $C_0^\infty((-T, -\tau/2))$, then $J_\theta(\mu; h) = O(h^N)$ for any $N \gg 1$ uniformly in $\mu \in I_0$.*

LEMMA 3.3. *There exists $T_0 > 0$ such that if $|t| > T_0$, then $\mathrm{Tr}(G(t; h) W) = O(h^N)$ for any $N \gg 1$.*

We proceed with the proof of the theorem, accepting these lemmas as proved.

(3) LEMMA 3.4. *$\rho'(\mu; h) = O(h^{-n-3})$ uniformly in $\mu \in I_0$ (and hence $\mu \in R^1$).*

For the proof of this lemma, we use two lemmas.

LEMMA 3.5. *Assume $(V)_\rho$ with $\rho > 0$ and that $\mu \in I_0$ is non-trapping. Then, for any $\alpha > \frac{1}{2}$,*

$$\| \langle x \rangle^{-\alpha} R(\mu \pm i0; H(h)) \langle x \rangle^{-\alpha} \| = O(h^{-1})$$

uniformly in $\mu \in I_0$, where $\| \;\|$ denotes the operator norm when considered as an operator from $L^2(R_x^n)$ into itself.

The above lemma has already been proved in [20], where we have used this resolvent estimate to study the semi-classical asymptotics for total scattering cross-sections. This lemma plays an important role in the proof of this theorem also.

LEMMA 3.6. *Let $\phi_+(x, \mu, \omega; h)$ be the out-going generalized eigenfunction of $H(h)$. Define*

$$\tilde{\phi}(x, \mu, \omega; \sigma, h) = \phi_+(x/\sigma, \mu\sigma^2, \omega; h), \qquad \sigma > 0.$$

Then

$$(\partial/\partial\sigma)\tilde{\phi}\,|_{\sigma=1} = -R(\mu + i0; H(h))\, U\phi_+,$$

where

$$U(x) = (\partial/\partial\sigma)(\sigma^{-2}V(x/\sigma))\,|_{\sigma=1} = -2V - (x \cdot \nabla)\, V.$$

Proof. We first note that $\phi_0(x/\sigma, \mu\sigma^2, \omega; h)$ is independent of σ. Hence $(\partial/\partial\sigma)\tilde{\phi}$ satisfies the out-going radiation condition. As is easily seen, $\tilde{\phi}$ obeys the equation

$$-\tfrac{1}{2}h^2\Delta\tilde{\phi} + \sigma^{-2}V(x/\sigma)\tilde{\phi} - \mu\tilde{\phi} = 0.$$

Hence, the desired relation can be obtained immediately. ∎

Proof of Lemma 3.4. We calculate $\rho'(\mu; h)$, using the relation

$$\rho'(\mu; h) = (2\mu)^{-1}(\partial/\partial\sigma)\rho(\mu\sigma^2; h)\,|_{\sigma=1}.$$

By definition,

$$\rho(\mu\sigma^2; h) = g(\mu\sigma^2)c_0(\mu\sigma^2, h)^2 \iint_{S^{n-1}} W(x)\,|\phi_+(x, \mu\sigma^2, \omega; h)|^2\, d\omega\, dx.$$

We make a change of variables $x \to y = \sigma x$ in the above integral and differentiate the resulting relation with respect to σ. Then Lemmas 3.5 and 3.6 yield the desired order estimate. ∎

(4) We now complete the proof of the theorem. We take $\theta_0 \in C_0^\infty((-1, 1))$ such that $\theta_0 = 1$ for t, $|t| < \frac{1}{2}$. Fix an integer $K \gg 1$ arbitrarily and set $\theta_K(t) = \theta_0(h^K t)$. Define

$$\phi_K(\tau; h) = (2\pi h)^{-1} \int \exp(ih^{-1}\tau t)\theta_0(h^K t)\, dt.$$

If we denote by $\hat{\theta}(\tau)$ the Fourier transform of $\theta(t)$, $\hat{\theta}(\tau) = \int \exp(-it\tau)\theta(t)\, dt$, then

$$\phi_K(\tau; h) = (2\pi h^{K+1})^{-1}\, \hat{\theta}_0(-h^{-(K+1)}\tau)$$

and also

$$\int \phi_K(\tau; h)\, d\tau = \theta_0(0) = 1.$$

By definition, we have

$$J_{\theta_K}(\mu; h) = \int \rho(\mu - \tau; h) \phi_K(\tau; h)\, d\tau$$

and by Lemmas 3.1–3.3, we see that $J_{\theta_K}(\mu; h)$ has an asymptotic expansion in h. Thus we have only to evaluate the difference between $\rho(\mu; h)$ and $J_{\theta_K}(\mu; h)$. By Lemma 3.4, this is estimated as

$$O(h^{-(K+1)}) O(h^{-(n+3)}) \int |\tau|\, |\hat{\theta}_0(-h^{-(K+1)}\tau)|\, d\tau = O(h^{K-n-2}).$$

This completes the proof. ∎

4. Proof of Lemmas 3.1–3.3

In this section we prove Lemmas 3.1–3.3. The method of proof is based on the calculus of oscillatory integral operators. We first introduce a certain class of symbols.

Symbol Class A_μ. For given $\Omega \subset R^n_x \times R^n_\xi$, we denote by $A_\mu(\Omega)$ the set of all $a(x, \xi)$, $(x, \xi) \in \Omega$, such that

$$|\partial_x^\alpha \partial_\xi^\beta a(x, \xi)| \leqslant C_{\alpha\beta N} \langle x \rangle^{\mu - |\alpha|} \langle \xi \rangle^{-N}$$

for any $N \gg 1$. If, in particular, $\Omega = R^n_x \times R^n_\xi$, then we write A_μ for $A_\mu(\Omega)$.

Most of the symbols we consider later have compact support in ξ and hence are of class $A_\mu(\Omega)$. We say that a family of symbols $a(x, \xi; \varepsilon)$ with parameter ε belongs to $A_\mu(\Omega)$ uniformly in ε, if the constants $C_{\alpha\beta N}$ above are taken uniformly in ε.

We again write $p(x, \xi) = \frac{1}{2}|\xi|^2 + V(x)$. Let $\{x(t; y, \eta), \xi(t; y, \eta)\}$ be the phase trajectory with initial state (y, η) associated with the hamiltonian function $p(x, \xi)$. We denote by Φ_t the canonical mapping

$$\Phi_t\colon (y, \eta) \to \{x(t; y, \eta), \xi(t\colon y, \eta)\}.$$

Proof of Lemma 3.1. The lemma is proved in the standard way based on short time parametrices for the Schrödinger equation. If, in particular, $W(x)$ is of compact support, the proof is done in exactly the same way as in [3, 8], etc. Even if $W(x)$ is not of compact support, any serious difficulty does not occur. We give only a sketch for the proof.

By Proposition 2.1, it suffices to prove the lemma for $\omega(x, hD_x)$ with symbol $\omega(x, \xi) \in A_0$ supported in $\{(x, \xi): p(x, \xi) \in I_0\}$, I_0 being the fixed non-trapping energy interval. We define

$$I_\theta(\mu; h) = (2\pi h)^{-1} \int \exp(ih^{-1}t\mu)\, \theta(t) \operatorname{Tr}(W \exp(-ih^{-1}tH(h))\omega(x, hD_x))\, dt$$

for $\mu \in I_0$. Let $S(t, x, \xi)$, $|t| < \tau \ll 1$, be the solution to the Hamilton–Jacobi equation $\partial_t S + p(x, \nabla_x S) = 0$ with $S|_{t=0} = \langle x, \xi \rangle$. The function S has the following property (S): If ξ ranges over a compact set, then $\partial_t^k \partial_x^\alpha \partial_\xi^\beta S$ with $k + |\alpha| + |\beta| \geqslant 2$ is bounded uniformly in (t, x, ξ), $x \in R_x^n$. This follows from the fact that S is the generating function of the canonical mapping Φ_t. By constructing a short time parametrix for $\exp(-ih^{-1}tH(h))$, $|t| < \tau$, we can write $I_\theta(\mu; h)$ in the form

$$(2\pi h)^{-(n+1)} \iiint \exp(ih^{-1}\psi(t, x, \xi))\theta(t)\, W(x) a_N(t, x, \xi; h)\, dx\, d\xi\, dt + O(h^N)$$

for any $N \gg 1$, where

$$\psi(t, x, \xi) = t\mu + S(t, x, \xi) - \langle x, \xi \rangle$$

and a_N belongs to A_0 uniformly in t, $|t| < \tau$, and h with support in $\{(x, \xi): p(x, \nabla_x S) \in I_0\}$. We apply the stationary phase method to the above integral. As is easily seen, the set of the stationary points of ψ is given by $\{(t, x, \xi): t = 0,\ p(x, \xi) = \mu\}$, because $\mu \in I_0$ is not a critical value of $p(x, \xi)$.

We first consider the case $W(x) \in C_0^\infty(R_x^n)$. We make a change of variables $z = p(x, \xi)$ and use the stationary phase method in the variables (t, z), regarding the other variables as parameters. These parameters range over a compact set. Since ψ behaves like $\psi = t\mu - tz + O(t^2)$ as $|t| \to 0$, the stationary point $(0, \mu)$ is non-degenerate. This proves the lemma in the case of compact support.

Next we consider the case of non-compact support. Assume that $W(x)$ has support in $\{x: |x| > R\}$ for $R \gg 1$. The above arguments apply to this case without any essential change but we have to look at the dependence on parameters carefully. We put

$$b_N(t, x, \xi; h) = \theta(t)\, W(x)\, a_N(t, x, \xi; h).$$

By partition of unity, we may assume that b_N has support in

$$\Sigma = \{(t, x, \xi): |t| < \tau, |x| > R, |\xi| < c, c^{-1} < |\xi_1| < c\}$$

for some $c > 1$. We set $\xi' = (\xi_2, ..., \xi_n)$ and make a change of variables $(t, x, \xi) \to (t, x, \xi', z)$ with $z = p(x, \xi)$. We denote by Ψ the representation of ψ in terms of the new variables. We assert that

$$|\partial_t \Psi| + |\partial_z \Psi| \geq c_0(|t| + |z - \mu|) \tag{4.1}$$

in Σ. By (4.1), we can apply the stationary phase method with parameters (x, ξ') to obtain the asymptotic expansion with a uniform remainder estimate. Assertion (4.1) is easy to prove. By a direct differentiation,

$$\partial_t \Psi = (\mu - p(x, \nabla_x S)) \,|_{p(x, \xi_1, \xi') = z},$$

$$\partial_z \Psi = \xi_1^{-1}((\partial/\partial\xi_1) S - x_1) \,|_{p(x, \xi_1, \xi') = z}.$$

By property (S), we can take τ so small that $|\partial_z \Psi| > c_1 |t|$ for $|t| < \tau$. By the energy conservation, we have

$$p(x, \nabla_x S(t, x, \xi)) - p(x, \xi) = \int_0^t (d/ds) V(\nabla_\xi S(s, x, \xi))\, ds$$

and hence we can take R so large that

$$|p(x, \nabla_x S(t, x, \xi)) - p(x, \xi)| < (c_1/2)\, |t|$$

for $|x| > R$. This proves (4.1) and the proof of lemma is complete. ∎

The next lemma reduces the proof of Lemmas 3.2 and 3.3 to the case $W(x) \in C_0^\infty(R_x^n)$.

LEMMA 4.1. *Let $W(x)$ be as in Theorem* 0.1 *and let τ be as in lemma* 3.1. *If $W(x)$ has support in $\{x: |x| > R_0\}$ for $R_0 \gg 1$, then* $\mathrm{Tr}(G(t; h) W) = O(h^N)$ *for any $N \gg 1$ uniformly in t, $|t| > \tau/2$.*

Proof. The proof uses the out-going parametrices constructed globally in time $t \geq 0$. In the Appendix, we will give a brief review on the construction of such parametrices based on the idea due to Isozaki and Kitada [11].

We consider the case $t > 0$ only. It suffices to prove the lemma for the following two types of symbols:

(a) $\omega_+(x, \xi) \in A_0$ is supported in

$$\{(x, \xi): |x| > R_0, p(x, \xi) \in I_0, \langle x, \xi \rangle > -\tfrac{1}{2} |x|\, |\xi|\};$$

(b) $\omega_-(x, \xi) \in A_0$ is supported in

$$\{(x, \xi): |x| > R_0,\ p(x, \xi) \in I_0,\ \langle x, \xi \rangle < \tfrac{1}{2}|x|\ |\xi|\}.$$

We define

$$d_\pm(t; h) = \mathrm{Tr}(W \exp(-ih^{-1}tH(h))\, \omega_\pm(x, hD_x))$$

for $t > \tau/2$. By Lemma A.1 in the Appendix, we have $d_+(t; h) = O(h^N)$ for any $N \gg 1$. On the other hand, by the cyclic property of trace, $d_-(t; h)$ can be rewritten as

$$d_-(t; h) = \overline{\mathrm{Tr}}(\bar{W} \exp(ih^{-1}tH(h))\, \omega_-(x, hD_x)^*), \qquad t > 0.$$

Hence, (A.4) in the Appendix proves $d_-(t; h) = O(h^N)$. Thus the proof is complete. ∎

By Lemma 4.1, we have only to prove Lemmas 3.2 and 3.3 in the case $W \in C_0^\infty(R_x^n)$. We keep the same notations and assumptions as in Lemmas 3.2 and 3.3.

LEMMA 4.2. *Assume that* $W(x) \in C_0^\infty(R_x^n)$. *Fix* $T \gg 1$ *arbitrarily. If* $\theta \in C_0^\infty((\tau/2, T))$ *or* $C_0^\infty((-T, -\tau/2))$, *then* $J_\theta(\mu; h) = O(h^N)$ *for any* $N \gg 1$ *uniformly in* $\mu \in I_0$.

Proof. We give only a sketch. The argument is based on the iteration of short time parametrices and also is standard. For details, see again [3, 8], etc.

We consider the case $\theta \in C_0^\infty((\tau/2, T))$ only. Assume that $W(x)$ is supported in $\{x: |x| < R\}$ for some R. It suffices to prove the lemma for $\omega(x, hD_x)$ with symbol $\omega(x, \xi) \in A_0$ supported in $\{(x, \xi): p(x, \xi) \in I_0, |x| < R\}$. We may assume that $\theta(t)$ is supported in $((k-1)\tau, (k+1)\tau)$ with some $k \geq 1$. For such θ, $(2\pi h)^{(k+1)n+1} J_\theta(\mu; h)$ is represented in the form

$$\iiint \exp(ih^{-1}\psi(t, x, \Theta, \xi))\theta(t)\, W(x) a_N(t, x, \Theta, \xi; h)\, dt\, dx\, d\Theta\, d\xi + O(h^N)$$

for any $N \gg 1$, where $\Theta = (x_1, \xi_1, ..., x_k, \xi_k) \in R^{2kn}$, $a_N \in C_0^\infty(R_t^1 \times R_x^n \times R_\Theta^{2kn} \times R_\xi^n)$, and

$$\psi = t\mu + S(t - k\tau, x, \xi_k) - \langle x, \xi \rangle + \sum_{j=1}^{k} \{S(\tau, x_j, \xi_{j-1}) - \langle x_j, \xi_j \rangle\}$$

with $\xi_0 = \xi$. We easily see that the stationary points of ψ lie in

$$\{(t, x, \Theta, \xi): p(x, \xi) = \mu,\ \Phi_t(x, \xi) = (x, \xi) \text{ for some } t \in \operatorname{supp} \theta\}.$$

By the non-trapping condition, the above set is void and hence the non-stationary phase method proves the lemma. ∎

LEMMA 4.3. *Assume that* $W(x) \in C_0^\infty(R_x^n)$. *Then there exists* $T \gg 1$ *such that if* $|t| > T$, *then* $\operatorname{Tr}(G(t; h) W) = O(h^N)$ *for any* $N \gg 1$.

Proof. The method of proof is based on the Egorov theorem and out-going parametrices. We consider the case $t > 0$ only. It again suffices to prove the lemma for $\omega(x, hD_x)$ as in Lemma 4.2. Set

$$B_T(h) = \exp(-ih^{-1}TH(h))\,\omega(x, hD_x)\,W \exp(ih^{-1}TH(h)).$$

Then, by the semi-classical Egorov theorem [19], we have

$$B_T(h) = \sum_{j=0}^{n+N} b_{jT}(x, hD_x)h^j + R_{NT}(h)$$

for any $N \gg 1$, where $R_{NT}(h)$ is of trace class with bound $\|R_{NT}(h)\|_{\mathrm{tr}} = O(h^N)$, while the symbol $b_{jT}(x, \xi) \in C_0^\infty(R_x^n \times R_\xi^n)$ has support in

$$\Omega_T = \{(x, \xi) : p(x, \xi) \in I_0,\ (x, \xi) = \Phi_T(t, \eta) \text{ for } (y, \eta) \in \operatorname{supp} \omega\}.$$

By the non-trapping condition, we can choose T so large that Ω_T is contained in the out-going region

$$\Omega_+ = \{(x, \xi) : p(x, \xi) \in I_0,\ |x| > R_1,\ \langle x, \xi \rangle > 0\}$$

for some $R_1 \gg 1$. Hence, by the cyclic property of trace, we have only to evaluate the trace of the form

$$d(t; h) = \operatorname{Tr}(\exp(-ih^{-1}tH(h))b(x, hD_x)), \qquad t > T,$$

where $b(x, \xi) \in C_0^\infty(R_x^n \times R_\xi^n)$ (and hence $\in A_{-N}$ for any $N \gg 1$) has support in Ω_+. Thus it follows from Lemma A.1 that $d(t; h) = O(h^N)$ for any $N \gg 1$ uniformly in $t > T$. This completes the proof. ∎

Lemmas 3.2 and 3.3 follow from Lemmas 4.1–4.3 at once.

5. Time Delay and Trace Formula

In this section we introduce the (average) time delay in quantum mechanics, following the idea due to [5], where total scattering cross sections have been introduced in the framework of the time-dependent scattering theory. We will show that it is natural to define this quantity by the λ-derivatives of spectral shift function in the Birman–Krein trace formula [2, 15]. The time delay problems in scattering processes have been studied by many authors. For related references, see [13] and the references quoted there. Among these references, the relation between the time delay and the trace formula has been discussed in [12].

We begin by introducing several notations. We denote by $|\ |_0$ the L^2 norm. Let $B_R = \{x: |x| < R\}$ and let $L^2(B_R) = \{f \in L^2: \operatorname{supp} f \subset B_R\}$. We also denote by χ_R the characteristic function of B_R. The probability of finding the state $\exp(-ih^{-1}tH_0(h))f$, $f \in L^2$, in $L^2(B_R)$ at time t is given by

$$|\chi_R \exp(-ih^{-1}tH_0(h))\, f|_0^2$$

and hence the total time spent in $L^2(B_R)$ is given by

$$T_{0R}(f) = \int |\chi_R \exp(-ih^{-1}tH_0(h)) f|_0^2\, dt.$$

We now consider a homogeneous beam of free particles incoming from the long distance with density one per unit area. We fix the incoming direction $\omega \in S^{n-1}$ and the energy $\lambda > 0$. Let $Y(\theta) = Y(\theta; \omega) \in C_0^\infty(S^{n-1})$ and $g(\mu) = g(\mu; \lambda) \in C_0^\infty((0, \infty))$ be supported in a small neighborhood of ω and λ, respectively. We denote by Π the hyperplane orthogonal to ω. For $a \in \Pi$, we define

$$g_a(\mu, \theta; \lambda, \omega, h) = \exp(-ih^{-1} \sqrt{2\lambda}\, \langle a, \theta \rangle)\, Y(\theta)\, g(\mu)$$

and

$$f_a(x; \lambda, \omega, h) = (F_0(h)^* g_a)(x),$$

where $F_0(h): L^2 \to L^2((0, \infty); L^2(S^{n-1}))$ is the unitary operator defined by (1.1) which gives the spectral representation for $H_0(h)$. We further define $S_{0R}(\lambda, \omega; h)$ by

$$S_{0R}(\lambda, \omega; h) = \int_\Pi T_{0R}(f_a)\, da.$$

We calculate S_{0R} formally, making use of the representation

$$\exp(-ih^{-1}tH_0(h)) f_a = \int_0^\infty \int_{S^{n-1}} \psi_0(x, \mu, \theta; h) \exp(-ih^{-1}t\mu)\, g_a(\mu, \theta)\, d\theta\, d\mu$$

and exchanging the order of integrations. We first carry out the t-integration,

$$\int \exp(-ih^{-1}t(\mu - \mu'))\, dt = (2\pi h)\delta(\mu - \mu'),$$

and then the a-integration,

$$\int_{\Pi} \exp(-ih^{-1}\sqrt{2\mu}\,\langle a, \theta-\theta'\rangle)\,da = (2\pi h)^{n-1}(2\mu)^{-(n-1)/2}\,\delta(\theta_1-\theta_1'),$$

where $\theta_1 = \theta - \langle\theta, \omega\rangle\omega \in \Pi$. Thus we obtain

$$S_{0R} = \int_0^\infty \int_{S^{n-1}} |g(\mu)|^2\,|Y(\theta)|^2\,\langle\theta, \omega\rangle^{-1}\,\eta_{0R}(\mu, \theta; h)\,d\theta\,d\mu,$$

where

$$\eta_{0R} = (2\mu)^{-1/2}\int_{B_R} |\phi_0(x, \mu, \theta; h)|^2\,dx.$$

In the limits $|Y(\theta;\omega)|^2 \to \delta(\theta-\omega)$ and $|g(\mu;\lambda)|^2 \to \delta(\mu-\lambda)$, the quantity $S_{0R}(\lambda, \omega; h)$ converges to $\eta_{0R}(\lambda, \omega; h)$, which represents the total time spent in B_R by a homogeneous beam of free particles incoming from the direction ω with energy λ.

We can calculate the corresponding quantity in classical mechanics. Let σ_n be the surface area of the n-dimensional unit sphere and let ω_n be again the volume of the n-dimensional unit ball. Then this quantity is calculated as

$$2\sigma_{n-2}(2\lambda)^{-1/2}\int_0^R (R^2-b^2)^{1/2}\,b^{n-2}\,db = \omega_n(2\lambda)^{-1/2}R^n,$$

which just coincides with $\eta_{0R}(\lambda, \omega; h)$, where b denotes the impact parameter.

For the perturbed system $H(h) = H_0(h) + V$, we introduce the quantity $S_R(\lambda, \omega; h)$ analogous to $S_{0R}(\lambda, \omega; h)$. Let $W_\pm(h)$ be the wave operators defined by

$$W_\pm(h) = s - \lim_{t\to\mp\infty} \exp(ih^{-1}tH(h))\exp(-ih^{-1}tH_0(h)).$$

Then we define $S_R(\lambda, \omega; h)$ by

$$S_R(\lambda, \omega; h) = \int_{\Pi}\int |\chi_R \exp(-ih^{-1}tH(h))\,W_+(h)\,f_a|_0^2\,dt\,da.$$

Recall the notations. L^2_{ac} is the absolutely continuous subspace of $H(h)$ and $F_\pm(h)\colon L^2_{\mathrm{ac}} \to L^2((0, \infty); L^2(S^{n-1}))$ is the unitary operator defined by (1.2) which gives the spectral representation for $H(h)$ restricted to L^2_{ac}. Since $W_+(h) = F_+(h)^* F_0(h)$, we have

$$\exp(-ih^{-1}tH(h))\, W_+ f_a$$
$$= \int_0^\infty \int_{S^{n-1}} \psi_+(x, \mu, \theta; h) \exp(-ih^{-1}t\mu)\, g_a(\mu, \theta)\, d\theta\, d\mu.$$

Thus, by a calculation similar to that used for S_{0R}, we obtain

$$S_R = \int_0^\infty \int_{S^{n-1}} |g(\mu)|^2\, |Y(\theta)|^2 \langle \theta, \omega\rangle^{-1} \eta_R(\mu, \theta; h)\, d\theta\, d\mu,$$

where

$$\eta_R = (2\mu)^{-1/2} \int_{B_R} |\phi_+(x, \mu, \theta; h)|^2\, dx.$$

Now, we take the difference between $\eta_R(\lambda, \omega; h)$ and $\eta_{0R}(\lambda, \omega, h)$ and average it over $\omega \in S^{n-1}$,

$$\tau_R(\lambda; h) = (\sigma_{n-1})^{-1} \int_{S^{n-1}} (\eta_R(\lambda, \omega; h) - \eta_{0R}(\lambda, \omega; h))\, d\omega.$$

Recall the representation (1.3) for the kernel $e'(x, y; \lambda, h)$ of $E'(\lambda; H(h))$. We denote by $e'_0(x, y; \lambda, h)$ the kernel of $E'(\lambda; H_0(h))$. Then we can rewrite $\tau_R(\lambda; h)$ as

$$\tau_R(\lambda; h) = (\sigma_{n-1})^{-1} (2\lambda)^{-1/2} c_0(\lambda, h)^{-2} \int_{B_R} (e'(x, x; \lambda, h)$$
$$- e'_0(x, x; \lambda, h))\, dx$$

with the normalized constant $c_0(\lambda, h)$ in Section 1. Hence it follows that

$$\mathrm{Tr}(\chi_R(f(H(h)) - f(H_0(h)))\,\chi_R) = \sigma_{n-1} \int_0^\infty f(\lambda)(2\lambda)^{1/2} c_0(\lambda, h)^2\, \tau_R(\lambda; h)\, d\lambda \tag{5.1}$$

for $f \in C_0^\infty((0, \infty))$.

We are interested in the problem of whether or not $\tau_R(\lambda; h)$ is convergent as $R \to \infty$. The Birman–Krein trace formula gives a partial answer to this problem.

THEOREM. *Assume $(V)_\rho$ with $\rho > n$. Then, for $f \in C_0^\infty(R^1)$, $f(H(h)) - f(H_0(h))$ is of trace class and there exists $\theta(\lambda; h) \in L^1_{\text{loc}}(R^1)$ uniquely such that: $\theta(\lambda; h) \to 0$ as $\lambda \to -\infty$;*

$$\det S(\lambda; h) = \exp(2\pi i \theta(\lambda; h)) \qquad \text{for} \quad \lambda > 0; \tag{5.2}$$

$$\operatorname{Tr}(f(H(h)) - f(H_0(h))) = -\int f'(\lambda)\, \theta(\lambda; h)\, d\lambda, \tag{5.3}$$

where $S(\lambda; h): L^2(S^{n-1}) \to L^2(S^{n-1})$ is the scattering matrix defined for the pair $(H_0(h), H(h))$.

Remark. The function $\theta(\lambda; h)$ is called the spectral shift function or the total scattering phase because of property (5.2).

The above theorem follows from the general theory of the Birman–Krein trace formula (see also [4, 7, 14], etc.).

By (5.1) and (5.3), $\tau_R(\lambda; h)$ is convergent to

$$\tau_\infty(\lambda; h) = (\sigma_{n-1})^{-1} (2\lambda)^{-1/2} c_0(\lambda, h)^{-2}\, \theta'(\lambda; h) \tag{5.4}$$

as $R \to \infty$ in the distribution sense (i.e., in $D'((0, \infty))$). Thus, we shall call $\tau_\infty(\lambda; h) \in D'((0, \infty))$ the (average) time delay for the pair $(H_0(h), H(h))$. We do not know whether or not $\tau_R(\lambda; h)$ is pointwise convergent as $R \to \infty$.

5. Asymptotics for Time Delay

In the previous section we have defined the time delay $\tau_\infty(\lambda; h) \in D'((0, \infty))$ in the distribution sense. The aim of the present section is twofold. First we show that $\theta(\lambda; h) \in C^1((0, \infty))$, which implies that $\tau_\infty(\lambda; h)$ is well-defined as a function, and establish the relation between $\tau_\infty(\lambda; h)$ and $e'(x, x; \lambda, h)$ through the representation for $\theta'(\lambda; h)$. Second, we apply Theorems 0.1 and 2.1 to obtain the semi-classical asymptotic formula as $h \to 0$ for $\tau_\infty(\lambda; h)$. We compare the leading term of the obtained asymptotic formula with the corresponding time delay in classical mechanics for a class of central potentials in the 3-dimensional space R^3_x. We can show that both quantities coincide with each other, if the energy λ under consideration is restricted to a non-trapping energy region. On the other hand, if λ is in a trapping energy region, both quantities do not necessarily coincide with each other.

We begin by proving the following

PROPOSITION 6.1. *Assume $(V)_\rho$ with $\rho > n$. Then $\theta(\lambda; h) \in C^1((0, \infty))$ and*

$$\theta'(\lambda; h) = -(2\lambda)^{-1} \int U(x) e'(x, x; \lambda, h)\, dx, \tag{6.1}$$

where $U(x)$ is defined in Lemma 3.6.

Proof. The proof is divided into several steps.

(0) We recall the properties of the scattering matrix $S(\lambda; h)$. For details, see [18]. Under the assumption $(V)_\rho$ with $\rho > n$, $S(\lambda; h)$, $\lambda > 0$, is a unitary operator acting on the space $L^2(S^{n-1})$ and takes the form $S(\lambda; h) = \mathrm{Id} - (2\pi i) T(\lambda; h)$ with T of trace class. The integral kernel $T(\theta, \omega; \lambda, h)$ of $T(\lambda; h)$ is given by

$$T(\theta, \omega; \lambda, h) = (V\psi_+(\cdot, \lambda, \omega; h), \psi_0(\cdot, \lambda, \theta; h)), \tag{6.2}$$

where (,) denotes the L^2 scalar product.

(1) We first consider the case in which $V(x)$ is of compact support. Assume that $V(x) \in C_0^\infty(R^n)$. Then we know from the arguments in [14] that $\theta(\lambda; h)$ is analytic in $\lambda > 0$ and also it follows from (5.2) that

$$\theta'(\lambda; h) = -\mathrm{Tr}(S(\lambda; h)(d/d\lambda) T(\lambda; h)^*).$$

(See [6, p. 163].) We calculate the above trace by a method similar to that in [10]. As in the proof of Lemma 3.4, we use the relation

$$(d/d\lambda) T(\lambda; h)^* = (2\lambda)^{-1} (\partial/\partial\sigma) T(\lambda\sigma^2; h)|_{\sigma=1}.$$

By (6.2), the kernel of $T(\lambda\sigma^2; h)^*$ is represented as

$$T^*(\theta, \omega; \lambda\sigma^2, h) = (\psi_0(\cdot, \lambda\sigma^2, \omega; h), V\psi_+(\cdot, \lambda\sigma^2, \theta; h)).$$

We make a change of variables $x \to y = \sigma x$ to obtain that

$$T^*(\theta, \omega; \lambda\sigma^2, h) = c_0(\lambda, h)^2\, (\phi_0(\cdot, \lambda, \omega; h), V(\cdot; \sigma)\, \tilde{\phi}(\cdot, \lambda, \theta; \sigma, h)),$$

where $V(x; \sigma) = \sigma^{-2} V(x/\sigma)$ and

$$\tilde{\phi}(x, \lambda, \theta; \sigma, h) = \phi_+(x/\sigma, \lambda\sigma^2, \theta; h).$$

Therefore, Lemma 3.6 yields

$$(\partial/\partial\sigma) T^*(\theta, \omega; \lambda\sigma^2, h)|_{\sigma=1} = c_0(\lambda, h)^2\, (U\phi_-(\cdot, \lambda, \omega; h), \phi_+(\cdot, \lambda, \theta; h)).$$

(2) It follows from the definition of $S(\lambda; h)$ that $S(\lambda; h)$ maps $\bar{\phi}_+(x, \lambda, \cdot; h)$ into $\bar{\phi}_-(x, \lambda, \cdot; h)$. This shows that

$$\mathrm{Tr}(S(\lambda; h)(d/d\lambda)T(\lambda; h)^*) = c_0(\lambda, h)^2 \iint_{S^{n-1}} U(x)\, |\phi_-(x, \lambda, \omega; h)|^2 \, d\omega\, dx$$

and hence the desired relation follows immediately from (1.3). Thus, the proof is complete in the case $V \in C_0^\infty(R^n)$.

(3) Next we consider the general case in which $V(x)$ is assumed to satisfy $(V)_\rho$ with $\rho > n$. For such a $V(x)$, the right side of (6.1) is well-defined. We denote by $s(\lambda; h)$ this term. We approximate $V(x)$ by a sequence of C_0^∞-potentials. Then, the standard limit procedure combined with the Birman–Krein trace formula and Theorem 4.3 of [1] gives the relation

$$-\int_0^\infty f'(\lambda)\theta(\lambda; h)\, d\lambda = \int_0^\infty f(\lambda)s(\lambda; h)d\lambda$$

for any $f \in C_0^\infty((0, \infty))$. This proves that $\theta(\lambda; h) \in C^1((0, \infty))$ and $\theta'(\lambda; h) = s(\lambda; h)$. Thus the proof is complete. ∎

We apply Theorems 0.1 and 2.1 with $W(x) = -U(x)$ to obtain the following

THEOREM 6.1. *Assume $(V)_\rho$ with $\rho > n$ and fix a bounded open interval $I \subset (0, \infty)$. If there are no critical values of $p(x, \xi) = \frac{1}{2}|\xi|^2 + V(x)$ in I, then $\tau_\infty(\lambda; h)$ defined by* (5.4) *has an asymptotic expansion in h,*

$$\tau_\infty(\lambda; h) \sim \sum_{j=0}^{\infty} \tau_{\infty j}(\lambda) h^j, \qquad h \to 0, \tag{6.3}$$

in the weak sense (i.e., in $D'(I)$), where

$$\tau_{\infty 0}(\lambda) = (2\lambda)^{-(n-1)/2} \int \{((2\lambda - 2V(x))_+)^{n/2-1} - (2\lambda)^{n/2-1}\}\, dx. \tag{6.4}$$

Furthermore, if the interval I is contained in a non-trapping energy region, then the asymptotic formula (6.3) *holds in the strong sense for $\lambda \in I$.*

Proof. Equation (6.3) is an immediate consequence of Proposition 6.1 and Theorems 0.1 and 2.1. We calculate the leading term $\tau_0(\lambda)$. By (5.4), we have

$$\tau_{\infty 0}(\lambda) = -(2\lambda)^{-(n+1)/2} \int U(x)((2\lambda - 2V(x))_+)^{n/2-1}\, dx.$$

If we note the relation

$$\nabla \cdot x\{2\lambda - 2V)_+^{n/2} - (2\lambda)^{n/2}\}$$
$$= n\{(2\lambda - 2V)_+^{n/2} - (2\lambda)^{n/2}\} - n(x \cdot \nabla V)((2\lambda - 2V)_+)^{n/2-1},$$

then (6.4) is obtained by a direct calculation. ▮

We shall calculate the corresponding quantity $\tau_{\mathrm{cl}}(\lambda)$ in classical mechanics for a class of central potentials in R_x^3. Assume that $V(x) = V(r)$, $r = |x|$, is a central potential satisfying $(V)_\rho$ with $\rho > 3$. Let b denote the impact parameter. Then, by the conservation law of energy and angular momentum, we have

$$\tfrac{1}{2}(\dot{r}^2 + l^2/r^2) + V(r) = \lambda$$

with $l = \sqrt{2\lambda} b$. We define $r(b; \lambda)$ by

$$r(b; \lambda) = \sup\{r\colon 2\lambda - 2V(r) - (2\lambda b^2)/r^2 < 0\}$$

and denote by $b(r; \lambda)$ the inverse function of $r(b; \lambda)$,

$$b(r; \lambda) = (2\lambda)^{-1/2} r(2\lambda - 2V(r))^{1/2},$$

for $r > r_0 = r(b; \lambda)|_{b=0}$. We take R large enough. Then the total time spent in $|x| < R$ is given by

$$I = 4\pi \int_0^{b_R} \int_{r_b}^R (2\lambda - 2V(r) - (2\lambda b^2)/r^2)^{-1/2}\, b\, dr\, db$$

with $b_R = b(R; \lambda)$ and $r_b = r(b; \lambda)$. We calculate the above integral, exchanging the order of integrations,

$$I = 4\pi(2\lambda)^{-1} \int_{r_0}^R (2\lambda - 2V(r))^{1/2} r^2\, dr.$$

Thus the classical quantity $\tau_{\mathrm{cl}}(\lambda)$ is given by

$$\tau_{\mathrm{cl}}(\lambda) = \lim_{R \uparrow \infty} \left[4\pi(2\lambda)^{-1} \left\{ \int_{r_0}^R (2\lambda - 2V(r))^{1/2} r^2\, dr - \int_0^R (2\lambda)^{1/2} r^2\, dr \right\} \right].$$

As is easily seen, if λ is in a non-trapping energy region, then both the quantities $\tau_{\infty 0}(\lambda)$ and $\tau_{\mathrm{cl}}(\lambda)$ coincide with each other. On the other hand, if λ is in a trapping energy region and if λ is not a critical value of $\frac{1}{2}|\xi|^2 + V(x)$, then both quantities are not expected to coincide with each other.

APPENDIX: OUT-GOING PARAMETRICES

In this appendix we give a brief review on the construction of out-going parametrices due to Isozaki and Kitada [11] (see also Section 5 in [20]).

We first fix the notations. For given (σ, d), $-1<\sigma<1$, $d>1$, let

$$\Gamma_+(\sigma, R, d)=\{(x, \xi): x\in\Sigma_+(\sigma, R; \xi), d^{-1}<|\xi|<d\},$$

where

$$\Sigma_+(\sigma, R; \xi)=\{x: |x|>R, \langle x, \xi\rangle>\sigma\,|x|\cdot|\xi|\}$$

for $R\gg 1$. Throughout the entire discussion, the potential $V(x)$ is assumed to satisfy $(V)_\rho$ with $\rho>0$. We may assume that $0<\rho<1$, which loses no generality. We further assume ξ to range over $\{\xi: d_0^{-1}<|\xi|<d_0\}$ for some $d_0>1$. Then, by Proposition 2.4 of [11], we can construct a real C^∞-smooth function $\phi(x, \xi)$ with the following properties: For given σ_0, there exists $R_0\gg 1$ such that: (i) $\phi(x, \xi)$ solves

$$\tfrac{1}{2}\,|\nabla_x\phi|^2+V(x)=\tfrac{1}{2}\,|\xi|^2$$

in $\Gamma_+(\sigma_0, R_0, d_0)$; (ii) $\phi(x, \xi)-\langle x, \xi\rangle$ belongs to $A_{1-\rho}$ (see Section 4 for the notation A_μ); (iii) $\phi(x, \xi)$ satisfies $|(\partial^2\phi/\partial x_j\,\partial\xi_k)-\delta_{jk}|<c(R_0)$, δ_{jk} being the Kronecker notation, where $c(R_0)$ can be made as small as we desire by taking R_0 sufficiently large.

For given $a(x, \xi)\in A_\mu$, we define $I_\phi(a; h)$: $S(R^n_x)\to S(R^n_x)$ by

$$(I_\phi(a; h)\,f)(x)=(2\pi h)^{-n}\iint \exp(ih^{-1}(\phi(x, \xi)-\langle y, \xi\rangle))\,a(x, \xi)\,f(y)\,dy\,d\xi.$$

For the above triplet (σ_0, R_0, d_0), we take σ_j, R_j, and d_j, $1\leqslant j\leqslant 3$, as follows: $\sigma_3>\sigma_2>\sigma_1>\sigma_0$, $R_3>R_2>R_1>R_0$, and $d_3<d_2<d_1<d_0$. Let $\omega(x, \xi)\in A_0$ be supported in $\Gamma_+(\sigma_3, R_3, d_3)$. We shall construct a parametrix (approximate representation) globally in time $t\geqslant 0$ for the operator

$$U(t; h, \omega)=\exp(-ih^{-1}tH(h))\,\omega(x, hD_x), \qquad t\geqslant 0, \tag{A.1}$$

in the above form of oscillatory integral operators.

We first determine the symbol $a(x, \xi; h)$ to satisfy

$$\exp(-ih^{-1}\phi)(-\tfrac{1}{2}h^2\Delta+V-\tfrac{1}{2}\,|\xi|^2)\exp(ih^{-1}\phi)\,a\sim 0$$

asymptotically as $h \to 0$. If we set $a \sim \sum_{j=0}^{\infty} a_j(x, \xi) h^j$ formally, then $a_j(x, \xi)$ is inductively determined by solving the transport equation,

$$\begin{aligned} &\nabla_x \phi \cdot \nabla_x a_0 + \tfrac{1}{2}(\Delta_x \phi) a_0 = 0, \\ &\nabla_x \phi \cdot \nabla_x a_j + \tfrac{1}{2}(\Delta_x \phi)\, a_j - i\tfrac{1}{2} \Delta_x a_{j-1} = 0, \qquad j \geqslant 1, \end{aligned} \tag{A.2}$$

under the condition $a_0 \to 1$, $a_j \to 0$, $j \geqslant 1$, as $|x| \to \infty$. We can construct the solution $a_j \in A_{-j}(\Gamma_+(\sigma_1, R_1, d_1))$ to Eq. (A.2) in the region $\Gamma_+(\sigma_1, R_1, d_1)$ by the standard characteristic curve method and we extend a_j over the whole space $R_x^n \times R_\xi^n$ in the following way: (i) $a_j \in A_{-j}$; (ii) a_j has support in $\Gamma_+(\sigma_0, R_0, d_0)$.

We fix N arbitrarily and sufficiently large. We set

$$a_N(x, \xi; h) = \sum_{j=0}^{N} a_j(x, \xi) h^j$$

and

$$r_N(x, \xi; h) = h^{-(N+2)} \exp(-ih^{-1}\phi)(\tfrac{1}{2}h^2\Delta - V + \tfrac{1}{2}|\xi|^2) \exp(ih^{-1}\phi) a_N.$$

Then, by construction of ϕ and a_j, $j \geqslant 0$, it follows that $h^{N+1} r_N \in A_{-1}$ and $r_N \in A_{-(N+2)}(\Gamma_+(\sigma_1, R_1, d_1))$ uniformly in h. Let $\omega(x, \xi) \in A_0$ be as in (A.1). By the composite formula of Fourier integral operators, we can find $b_N(x, \xi; h) \in A_0$ with support in $\Gamma_+(\sigma_2, R_2, d_2)$ such that

$$\omega(x, hD_x) = I_\phi(a_N; h)(I_\phi(b_N; h))^* + h^N \omega_N(x, hD_x; h)$$

with $\omega_N \in A_{-N}$ (uniformly in h). We now define $U_N(t; h)$ and $R_N(t; h)$, $t \geqslant 0$, as

$$\begin{aligned} U_N(t; h) &= I_\phi(a_N; h) \exp(-ih^{-1}tH_0(h))(I_\phi(b_N; h))^*; \\ R_N(t; h) &= I_\phi(r_N; h) \exp(-ih^{-1}tH_0(h))(I_\phi(b_N; h))^*. \end{aligned}$$

Then, the Duhamel principle yields

$$U(t; h, \omega) = U_N(t; h) + h^N \exp(-ih^{-1}tH(h))\, \omega_N + h^{N+1} G_N(t; h), \tag{A.3}$$

where

$$G_N(t; h) = \int_0^t \exp(-ih^{-1}(t-s) H(h)) R_N(s; h)\, ds.$$

LEMMA A.1. *Let $W(x)$ satisfy $(V)_\rho$ with $\rho > n$. Then, for given (σ, d), there exists $R \gg 1$ such that if $\omega(x, \xi) \in A_0$ has suport in $\Gamma_+(\sigma, R, d)$, then*

$$\operatorname{Tr}(\exp(-ih^{-1}tH(h))\,\omega(x, hD_x)\,W) = O(h^N)$$

for any $N \gg 1$ uniformly in $t > \tau$, τ, $0 < \tau \ll 1$, being fixed arbitrarily.

Proof. The proof uses the representation (A.3). We can prove $\|G_N(t; h)\|_{\mathrm{tr}} = O(h^{-N/2})$ uniformly in $t \geqslant 0$ (see Lemma 5.1 in [20]). We assert that $\operatorname{Tr}(WU_N(t; h)) = O(h^N)$ for $t > \tau$. We can represent the above trace as

$$(2\pi h)^{-n} \iint \exp(-ih^{-1}t\,|\xi|^2/2)\,W(x)\,a_N(x, \xi, h)\,\bar{b}_N(x, \xi; h)\,dx\,d\xi$$

with a_N and $b_N \in A_0$ (uniformly in h). Hence, integrating by parts in ξ proves the lemma and the proof is complete. ∎

We fix another notation,

$$\Gamma_-(\sigma, R, d) = \{(x, \xi) \colon x \in \Sigma_-(\sigma, R; \xi),\ d^{-1} < |\xi| < d\},$$

where

$$\Sigma_-(\sigma, R; \xi) = \{x \colon |x| > R,\ \langle x, \xi \rangle \langle \sigma\,|\xi| \cdot |x|\}.$$

Let $\omega(x, \xi) \in A_0$ be supported in $\Gamma_-(\sigma, R, d)$ for $R \gg 1$. Then we can repeat the same arguments as above to prove that

$$\operatorname{Tr}(\exp(-ih^{-1}tH(h))\,\omega(x, hD_x)\,W) = O(h^N) \tag{A.4}$$

for any $N \gg 1$ uniformly in $t < -\tau$.

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