Uniform semiclassical approximation for two surfaces

I. DEFINITIONS

Functions $q_1(t)$ and $p_1(t)$ are defined as solutions of classical equations of motion in phase space,

$$\dot{q}_1(t) = p_1(t)/m, \quad \dot{p}_1(t) = -V_1'(q_1(t)), \tag{1}$$

with an initial condition

$$q_1(0) = x_0, \quad p_1(0) = P_1(x_0), \tag{2}$$

where

$$P_1(x) = \left[2m(E - V_1(x))\right]^{1/2}. \tag{3}$$

The phase function is defined as

$$f_1(x,t) = i\gamma(t)(x - q_1(t))^2 + p_1(t)(x - q_1(t)) + s_1(t), \tag{4}$$

where $\gamma(t)$ is some function, and $s_1(t)$ is a solution of a differential equation $\dot{s}_1(t) = p_1^2(t)/m$ with an initial condition $s_1(0) = 0$.

The pre-factor is defined as

$$c_1(t) = \left[\dot{p}_1(t) - 2i\gamma(t)\dot{q}_1(t)\right]. \tag{5}$$

Two basis functions ϕ_1 and ϕ_2 are some functions of x and $\boldsymbol{r}$. It is sufficient to know for the present study regarding these functions that $\boldsymbol{r} \mapsto \phi_1(x,\boldsymbol{r})$ and $\boldsymbol{r} \mapsto \phi_2(x,\boldsymbol{r})$ are linearly independent functions of $\boldsymbol{r}$ for any given x, and that

$$\phi_1'(x,\boldsymbol{r}) = g\,\theta'(x)\phi_2(x,\boldsymbol{r}), \quad \phi_2'(x,\boldsymbol{r}) = -g\,\theta'(x)\phi_1(x,\boldsymbol{r}), \tag{6}$$

where derivative is in respect to x, θ is some function, and g is a small coupling parameter.

The potential operator $\hat{V}$ is defined as a functional that when applied to any function in the form of $\alpha(x)\phi_1(x,\boldsymbol{r}) + \beta(x)\phi_2(x,\boldsymbol{r})$ gives $V_1(x)\alpha(x)\phi_1(x,\boldsymbol{r}) + V_2(x)\beta(x)\phi_2(x,\boldsymbol{r})$.

II. ZERO-ORDER TERM

The leading term of small-coupling expansion is constructed as

$$\Psi_{\mathrm{Z}}(x,\boldsymbol{r}) = \phi_1(x,\boldsymbol{r}) \int_{-\infty}^{\infty} \psi_1(x,t)dt, \tag{7}$$

where

$$\psi_1(x,t) = c_1(t) e^{\frac{i}{\hbar} f_1(x,t)}. \tag{8}$$

III. TESTING ZERO-ORDER TERM

We are testing that if $g = 0$ and $\Psi = \Psi_{\rm Z}$ then the Schrödinger equation

$$-\frac{\hbar^2}{2m}\Psi'' + (\hat{V} - E)\Psi = 0 \tag{9}$$

is valid at least in zero and first orders in $\hbar$. Since action of $\hat{V}$ on a function (7) with only first non-zero component reduces to multiplication of this function by $(E - P_1^2(x)/2/m)$, equation (9) is equivalent to

$$\hbar^2 \Psi_{\rm Z}''(x, \boldsymbol{r}) + P_1^2(x)\Psi_{\rm Z}(x, \boldsymbol{r}) = 0. \tag{10}$$

Taking into account that in the limit of zero coupling ($g = 0$) $\psi_1'(x) = 0$, equation (10) reduces to

$$\int_{-\infty}^{\infty} c_1(t) \left[\hbar^2 \psi_1''(x,t) + P_1^2(x)\psi_1(x,t)\right] dt = 0. \tag{11}$$

One of methods of verifying equation (10) is changing of variable of integration from time to coordinate and subsequent estimation of the integral by method of stationary phase. It could be done when there is no turning points, and when there is one to one correspondence between t and a coordinate variable x_1. Then, equation (11) is equivalent to

$$\int_{-\infty}^{\infty} \frac{m}{P(x_1)} C(x_1) \left[\hbar^2 \Psi''(x, x_1) + P^2(x)\Psi(x, x_1)\right] dx_1 = 0, \tag{12}$$

where the factor $m/P(x_1)$ is Jacobian of transformation equal to reciprocal velocity at point x_1, $P(x_1) = P_1(x_1)$,

$$\begin{aligned} \Psi(x, x_1) &= C(x_1)\, e^{\frac{i}{\hbar} F(x,x_1)}, && (13)\\ C(x_1) &= \left[\frac{P(x_1)}{m}(P'(x_1) - 2i\Gamma(x_1))\right]^{1/2}, && (14)\\ F(x, x_1) &= i\Gamma(x_1)(x - x_1)^2 + P(x_1)(x - x_1) + S(x_1), && (15) \end{aligned}$$

$\Gamma(x_1) = \gamma(q^{-1}(x_1))$, $S(x_1)$ is a solution of a differential equation $S'(x_1) = P(x_1)$ with an initial condition $S(x_0) = 0$. Leaving only the terms of zero and first order in $\hbar$, we rewrite l.h.s. of equation (12) as

$$I_0 + \hbar I_1 = \int_{-\infty}^{\infty} \left[R_0(x, x_1) + \hbar R_1(x, x_1)\right] e^{\frac{i}{\hbar} F(x,x_1)} dx_1, \tag{16}$$

where

$$R_0(x,x_1) = \frac{m}{P(x_1)} C(x_1) \left\{ -\left[F'_x(x,x_1)\right]^2 + P^2(x_1) \right\}, \tag{17}$$

$$R_1(x,x_1) = \frac{m}{P(x_1)} C(x_1) \left[iF''_{xx}(x,x_1) \right]. \tag{18}$$

Firstly, let us calculate $I_0 = \int_{-\infty}^{\infty} R_0(x,x_1) e^{\frac{i}{\hbar}F(x,x_1)} dx_1$ by method of stationary phase (including first-order correction). We expand functions entering this integral around the stationary point at $x_1 = x$:

$$F(x,x_1) = b_0 + b_2(x_1-x)^2 + b_3(x_1-x)^3 + \ldots, \tag{19}$$

$$R_0(x,x_1) = a_1(x_1-x) + a_2(x_1-x)^2 + \ldots, \tag{20}$$

where

$$b_0 = S(x), \quad b_2 = i\Gamma(x) - \tfrac{1}{2}P'(x), \quad b_3 = i\Gamma'(x) - \tfrac{1}{3}P''(x) \tag{21}$$

$$a_1 = 2C(x)P(x)\left[2i\Gamma(x) - P'(x)\right], \tag{22}$$

$$a_2 = 2C(x)\left\{2\Gamma^2(x) + i\Gamma(x)P'(x) + P(x)\left[3i\Gamma'(x) - P''(x)\right]\right\}. \tag{23}$$

Now, changing variable of integration $x_1 \to \xi = b_2^{1/2}(x_1 - x)$ and expanding integrand in powers of $\hbar$, it is straightforward to find that

$$I_0 = e^{\frac{i}{\hbar}b_0} \left(\frac{i\pi\hbar}{b_2}\right)^{1/2} \left[i\left(\frac{a_2}{2b_2} - \frac{3a_1b_3}{4b_2^2}\right)\hbar + O(\hbar^2) \right]. \tag{24}$$

After substitution of coefficients of expansions (21) - (23) into (24) we obtain

$$I_0 = e^{\frac{i}{\hbar}S(x)} \left(\frac{i\pi\hbar}{i\Gamma(x) - \frac{1}{2}P'(x)}\right)^{1/2} \left[2C(x)\Gamma(x)\hbar + O(\hbar^2)\right]. \tag{25}$$

Calculation of the integral $I_1 = \int_{-\infty}^{\infty} R_1(x,x_1) e^{\frac{i}{\hbar}F(x,x_1)} dx_1$ is performed by similar way, but only in zero order in $\hbar$. The pre-factor function is expanded in Taylor series around $x_1 = x$:

$$R_1(x,x_1) = d_0 + O(x_1 - x), \quad d_0 = -2C(x)\Gamma(x), \tag{26}$$

and the result of integration is

$$I_1 = e^{\frac{i}{\hbar}S(x)} \left(\frac{i\pi\hbar}{i\Gamma(x) - \frac{1}{2}P'(x)}\right)^{1/2} \left[-2C(x)\Gamma(x) + O(\hbar)\right]. \tag{27}$$

Finally, we calculate the total integral $I_0 + \hbar I_1$ using equations (25) and (27). Terms proportional to $\hbar$ cancel.

The first non-zero term in $\hbar$-expansion of (12) has order $\sim \hbar^2$. Its calculation could be performed in a similar way, but keeping two extra terms in Taylor expansions in powers of $x_1 - x$. The result is

$$I = e^{\frac{i}{\hbar}S(x)} \left(\frac{i\pi\hbar}{i\Gamma(x) - \frac{1}{2}P'(x)} \right)^{1/2} \left[-\frac{iR}{12P^2(x)C^7(x)}\hbar^2 + O(\hbar^2) \right], \tag{28}$$

where R is a lengthy polynomial in $P(x)$, $\Gamma(x)$ and their derivatives,

$$\begin{aligned} R &= (576\Gamma'(x)^3 + 576iP''(x)\Gamma'(x)^2 - 6(29P''(x)^2 + 2(2\Gamma(x) + iP'(x))(24\Gamma''(x) \\ &+ 5iP^{(3)}(x)))\Gamma'(x) - 15iP''(x)^3 - 192i\Gamma(x)\Gamma''(x)P''(x) + 96P'(x)\Gamma''(x)P''(x) \\ &+ 96\Gamma(x)^2\Gamma^{(3)}(x) - 24P'(x)^2\Gamma^{(3)}(x) + 96i\Gamma(x)P'(x)\Gamma^{(3)}(x) + 32\Gamma(x)P''(x)P^{(3)}(x) \\ &+ 16iP'(x)P''(x)P^{(3)}(x) + 3i(2\Gamma(x) + iP'(x))^2P^{(4)}(x))P(x)^3 + 12(2\Gamma(x) + iP'(x))(8P'(x)\Gamma'(x)^2 \\ &- 3(2\Gamma(x) - iP'(x))P''(x)\Gamma'(x) - 2i\Gamma(x)P''(x)^2 - 2(2\Gamma(x) + iP'(x))P'(x)\Gamma''(x) + \Gamma(x)(2\Gamma(x) \\ &+ iP'(x))P^{(3)}(x))P(x)^2 + 3(2\Gamma(x) + iP'(x))^2(14\Gamma'(x)P'(x)^2 - i(8\Gamma(x)^2 \\ &- 8iP'(x)\Gamma(x) + P'(x)^2)P''(x))P(x) + 9(2\Gamma(x) + iP'(x))^3P'(x)^2(2i\Gamma(x) + P'(x)). \end{aligned} \tag{29}$$

If $\Gamma(x)$ satisfies a differential equation $R = 0$, then the term $\sim \hbar^2$ is zero too.

IV. FIRST-ORDER WAVE FUNCTION

Up to the first order in coupling constant g, a guessed expression for the wave function is

$$\Psi(x, \boldsymbol{r}) = \Psi_{\mathrm{Z}}(x, \boldsymbol{r}) + g\Psi_{\mathrm{T}}(x, \boldsymbol{r}), \tag{30}$$

where the additional "transmission" term ("reflection" term will be added and discussed later) is

$$\Psi_{\mathrm{T}}(x, \boldsymbol{r}) = \phi_2(x, \boldsymbol{r}) \int_{-\infty}^{\infty} dt \int_0^t dt_1 \psi_{\mathrm{T}}(x, t, t_1), \tag{31}$$

$$\psi_{\mathrm{T}}(x, t, t_1) = c_{\mathrm{T}}(t, t_1) e^{\frac{i}{\hbar} f_{\mathrm{T}}(x,t,t_1)}. \tag{32}$$

The phase function $f_{\mathrm{T}}(x, t, t_1)$ in equation (32) is

$$t f_{\mathrm{T}}(x, t, t_1) = i\gamma(t)(x - q_{\mathrm{T}}(t, t_1))^2 + p_{\mathrm{T}}(t, t_1)(x - q_{\mathrm{T}}(t, t_1)) + s_{\mathrm{T}}(t, t_1), \tag{33}$$

the trajectory in phase space is defined as

$$q_{\mathrm{T}}(t,t_1) = Q_2(Q_1(x_0,t_1),t-t_1), \quad p_{\mathrm{T}}(t,t_1) = P_2(Q_1(x_0,t_1),t-t_1), \tag{34}$$

and the composite classical action is defined as

$$s_{\mathrm{T}}(t,t_1) = s_1(t_1) + \tfrac{1}{m}\int_{t_1}^{t} dt' P_2^2(Q_1(x_0,t_1),t'-t_1). \tag{35}$$

In equations (34) and (35), $Q_i(x,t)$ and $P_i(x,t)$ are classical trajectories in phase space on the i-th surface with an initial condition $Q_i(x,0) = x$ and $P_i(x,0) > 0$. The absolute value of $P_i(x,0)$ is determined from conservation of energy, $P_i^2(x,0)/2/m + V_i(x) = E$.