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On the equivalence of the classical-limit scattering matrix to the Wentzel–Kramers–Brillouin formalism

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Abstract. The classical-limit scattering matrix (CLSM) formalism was developed by Miller as a simple semiclassical procedure for the analyses of complex scattering and reaction processes. It invokes simple classical dynamics to define trajectories and superposition procedures to obtain interference effects. In one-dimensional systems, Miller has shown that the CLSM is equivalent to the standard WKB approximation. In this paper, it is shown that the equivalence between the CLSM and WKB extends to general systems. This equivalence between the WKB and CLSM formalisms is attributed to the general equivalence of the $\hbar$-expansion procedure in the WKB with the stationary phase approximation used in the CLSM.

1. Introduction

Since its development by Miller (1970, 1974), the classical-limit scattering matrix (CLSM) has been applied rather sparingly in the study of molecular scatterings (Miller 1970, 1971, 1972, 1974) and also in some applications in heavy ion nuclear elastic and inelastic scatterings (Koeling and Malfliet 1975). By the appropriate use of classical dynamics to treat both the translational as well as the internal degrees of freedom of a collisional system and further imposing the principle of quantum superposition, the CLSM is able to reproduce the quantal interference and diffractive features of a scattering event. However, in actual practice, the method involves searching for acceptable classical trajectories which satisfy both the initial and final quantum conditions of the scattering event. This is numerically not much simpler than the usual procedure adopted in scattering and reaction theories (Frobrich *et al* 1977).

In recent developments of the semiclassical distorted-wave Born approximation (DWBA) theory (Hasan and Brink 1978, Monaco and Brink 1985, Wong *et al* 1988, Wong and Low 1989, 1990), it has been shown that the use of various CLSM procedures combined with the WKB method have led to important simplifications of the DWBA theory. This renders the semiclassical DWBA theory feasible for extension to other more complex heavy-ion scattering reactions. It is thus necessary to re-examine various aspects of the relationship of the CLSM with the Wentzel–Kramers–Brillouin (WKB) formalism. In a one-dimensional system, the equivalence of the CLSM to the WKB formalism has been established by Miller (1974). This naturally raises the question whether the equivalence between the WKB and CLSM extends to general systems.

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In this paper, the development of both the CLSM and WKB will be traced starting from Dirac's transformation theory. In the process, the relationship between the $\hbar$-expansion procedure adopted in the WKB approximation with the stationary phase approximation (SPA) used in the CLSM is clarified. The general equivalence of the two formalisms is also established.

2. Quantum mechanical development of the CLSM and WKB formalisms in the classical limit of transformation theory

In the transformation theory of Dirac (1927, 1933, 1945), the physical properties of a system are specified by the eigenvalues Q_i of the canonically conjugate dynamical variables $\hat{Q}_i \in \{\hat{q}, \hat{p}\}$, $i=0$ or 1, such that

$$\hat{Q}_i|Q_i\rangle = Q_i|Q_i\rangle \tag{1}$$

where the bras $\langle Q_i|$ and kets $|Q_i\rangle$ characterize the state of the system. There exists then a transformation operator $\mathscr{A}$ which links the bras of one set of dynamical variables $\hat{Q}_i \in \{\hat{q}, \hat{p}\}$ to the kets of another set of dynamical variables $\hat{P}_j \in \{\hat{Q}, \hat{P}\}$, $j=0$ or 1. In different (Q_i, P_j) representations, the transformation functions $\langle Q_i|P_j\rangle$ of the operator $\mathscr{A}$ can be written as follows:

$$\langle Q_i|P_j\rangle = A_{ij}(Q_i, P_j) \exp[\mathrm{i}\mathfrak{F}_{ij}(Q_i, P_j)/\hbar] \tag{2}$$

where $\mathfrak{F}_{ij}(Q_i, P_j)$ is the quantum phase function.

In adopting this formulation, Dirac (1945) was able to preserve a close analogy between the quantum transformation theory with the classical transformation theory. This is shown by the derivation of the quantal analogue to the canonical equations from equation (2). The resulting quantum canonical equations are obtained as

$$Q_{1-i} = (-1)^i \frac{\partial \mathfrak{F}_{ij}}{\partial Q_i}(Q_i, P_j) \qquad P_{1-j} = (-1)^{j+1} \frac{\partial \mathfrak{F}_{ij}}{\partial P_j}(Q_i, P_j) \tag{3}$$

for all the different combinations (i, j) of the subscripts $i, j \in \{0, 1\}$.

The transformation relations (Dirac 1927, 1945) between different transformation functions are given by

$$\langle Q_i|P_j\rangle = \int \langle Q_i|Q_{1-i}\rangle \, \mathrm{d}Q_{1-i}\langle Q_{1-i}|P_j\rangle \qquad i, j = 0 \text{ or } 1 \tag{4a}$$

and

$$\langle Q_i|P_j\rangle = \int \langle Q_i|P_{1-j}\rangle \, \mathrm{d}P_{1-j}\langle P_{1-j}|P_j\rangle \qquad i, j = 0 \text{ or } 1 \tag{4b}$$

together with the unitarity condition

$$\int \langle Q_i|P_j\rangle \, \mathrm{d}P_j\langle P_j|Q'_i\rangle = \delta(Q_i - Q'_i). \tag{5}$$

The different representatives of a dynamical variable B are linked to each other through the equation

$$\langle Q_i|B|Q'_i\rangle = \int\int \langle Q_i|P_j\rangle \, \mathrm{d}P_j\langle P_j|B|P'_j\rangle \, \mathrm{d}P'_j\langle P'_j|Q'_i\rangle \qquad i, j = 0 \text{ or } 1. \tag{6}$$

Corresponding to the eigenvalues q and p of the dynamical variables $\hat{q}$ and $\hat{p}$ respectively is the standard transformation function $\langle q|p\rangle$ which can be written as

$$\langle q|p\rangle=\frac{1}{\sqrt{2\pi}}\,\mathrm{e}^{-\mathrm{i}qp/\hbar}. \tag{7}$$

It can be shown (Dirac 1958) that the uncertainty principle is implicitly built into the above transformation function when the unitarity equation (5) is used.

Following Miller (1970, 1974), the semiclassical CLSM formalism is then developed by consistently applying the stationary phase approximation (Erdelyi 1956) to the transformation theory. This involves using the standard result for an integral with a highly oscillatory integrand (Erdelyi 1956)

$$\int_{-\infty}^{\infty} A(z)\exp\{\mathrm{i}\alpha f(z)\}\,\mathrm{d}z=A(z_0)\left(\frac{2\pi\mathrm{i}\alpha}{f''(z_0)}\right)^{1/2}\exp\{\mathrm{i}\alpha f(z_0)\} \tag{8}$$

where α is a large parameter and z_0 is the stationary point of the phase function which is obtained as the solution of the equation

$$f'(z_0)=0. \tag{9}$$

Thus, in the case of the transformation relation (4a), the SPA is applied to the following integral:

$$\int_{-\infty}^{\infty} A_{1-i,j}^{(Q_{1-i},P_j)}\exp(\mathrm{i}((-1)^i\mathfrak{F}_{i,1-i}(Q_i,Q_{1-i})+\mathfrak{F}_{1-i,j}(Q_{1-i},P_j))/\hbar)\,\mathrm{d}Q_{1-i}. \tag{10}$$

In this manner, the classical limit condition $\hbar\rightarrow 0$ has been incorporated into the transformation theory when the SPA is invoked, with Planck's constant $\hbar$ occurring in the denominator of the large parameter $\alpha=1/\hbar$.

On evaluation of the integral (10) using the stationary phase condition, it is readily shown that the quantum phase functions $\mathfrak{F}_{ij}$ obey the dynamical equations as given by

$$\mathfrak{F}_{ij}(Q_i,P_j)=(-1)^iQ_iQ_{1-i}+\mathfrak{F}_{1-i,j}(Q_{1-i},P_j) \tag{11}$$

and

$$(-1)^iQ_i+\frac{\partial\mathfrak{F}_{1-i,j}}{\partial Q_{1-i}}(Q_{1-i},P_j)=0. \tag{12}$$

A second pair of dynamical equations for the quantum phase functions $\mathfrak{F}_{ij}$ in the form of

$$\mathfrak{F}_{ij}(Q_i,P_j)=\mathfrak{F}_{i,1-j}(Q_i,P_{1-j})-(-1)^jP_{1-j}P_j \tag{13}$$

and

$$\frac{\partial\mathfrak{F}_{i,1-j}}{\partial P_{1-j}}(Q_i,P_{1-j})-(-1)^jP_j=0 \tag{14}$$

is derived from the other transformation relation (4b) using the same procedure as that of equations (11) and (12). These equations are identical with the dynamical equations of the classical generating functions F_{ij} (Goldstein 1950). This establishes the correspondence relation between the quantum phase function in the classical limit and the classical generating function

$$\mathfrak{F}_{ij}(Q_i, P_j) \xrightarrow{\hbar\to 0} F_{ij}(Q_i, P_j). \tag{15}$$

Furthermore, substitution of the expression (2) for the transformation function into the unitarity condition (5), followed by the expansion of the phase function to the first order as

$$\mathfrak{F}_{ij}(Q_i', P_j) \approx \mathfrak{F}_{ij}(Q_i, P_j) + (Q_i' - Q_i)\frac{\partial \mathfrak{F}_{ij}}{\partial Q_i} \tag{16}$$

produces the CLSM expression for the amplitude $A_{ij}(Q_i, P_j)$ in the form

$$|A_{ij}(Q_i, P_j)|^2 = (2\pi)^{-1}(\partial^2 \mathfrak{F}_{ij}/\partial Q_i \partial P_j) \tag{17}$$

after further manipulation.

With the result (17) and the correspondence relation (15), the transformation function is reduced to the form given by

$$\langle Q_i | P_j \rangle = \left(\frac{\partial^2 F_{ij}(Q_i, P_j)/\partial Q_i \partial P_j}{2\pi \mathrm{i}\hbar}\right)^{1/2} \exp(\mathrm{i}F_{ij}(Q_i, P_j)/\hbar). \tag{18}$$

To account for quantal interference effects, Miller (1970, 1974) then assumed that the contributions arising from all possible classical trajectories can be superposed to produce the CLSM expression

$$\langle Q_i | P_j \rangle = \sum_{\substack{\text{classical} \\ \text{trajectories}}} \left(\frac{\partial^2 F_{ij}(Q_i, P_j)}{\partial Q_i \partial P_j}\right)^{1/2} \exp(\mathrm{i}F_{ij}(Q_i, P_j)/\hbar). \tag{19}$$

The mean value $\langle B(q, p)\rangle$ of a quantum dynamical variable $B(\hat{q}, \hat{p})$ can then be given by

$$\langle B(q,p)\rangle = (2\pi\hbar)^{-n} \iint \left|\frac{\partial^2 F_{ij}}{\partial Q_i \partial P_j}\right| B\left(Q_i', \frac{-\partial F_{ij}}{\partial P_j}\right) \times \exp\{\mathrm{i}P_i(Q_i' - Q_i)\}\, \mathrm{d}Q_i'\, \mathrm{d}Q_i \tag{20}$$

which on integration and using the Dirac delta function $\delta(Q_i' - Q_i)$ reduces to

$$\langle B(q,p)\rangle = \int \left|\frac{\partial^2 F_{ij}}{\partial Q_i \partial P_j}\right| B\left(Q_i, \frac{-\partial F_{ij}}{\partial P_j}\right) \mathrm{d}Q_i. \tag{21}$$

The correspondence relation between the mean value of a quantum dynamical variable in the classical limit and its classical analogue is thus stated by

$$\langle B(q,p)\rangle \xrightarrow{\hbar\to 0} \int \left|\frac{\partial^2 F_{ij}}{\partial Q_i \partial P_j}\right| B\left(Q_i, \frac{-\partial F_{ij}}{\partial P_j}\right) \mathrm{d}Q_i. \tag{22}$$

With these correspondence relations, it has been shown that in principle the CLSM formalism allows all degrees of freedom in a collisional system to be treated classically. Conceptually, this is an important advance in scattering theory as it provides a classical-like picture of scattering processes and greatly simplifies the computation of the dynamical parameters involved. Combined with the principle of superposition of contributions from the various classical trajectories, the CLSM is then able to reproduce the quantal interference and diffractive effects of heavy ion nuclear elastic and inelastic scattering (Koeling and Malfliet 1975), thus making it a potentially powerful numerical tool. Nevertheless, before the CLSM is successfully extended to more complex nuclear reactions it is necessary to find methods which enable the complete determination of the contributing classical trajectories for systems with many degrees of freedom (Frobrich *et al* 1977).

With respect to one-dimensional systems, Miller (1974) has shown that the transformation functions (19) reduces to the expression given by

$$\langle x|E\rangle = (2\pi\hbar)^{1/2}\left(\frac{2(E-V(x))}{m}\right)^{1/4}\left\{\exp\left(\frac{-\mathrm{i}\pi}{4}+\frac{\mathrm{i}}{\hbar}\int \mathrm{d}x(2m(E-V(x)))^{1/2}\right)\right.$$
$$\left.+\exp\left(\frac{\mathrm{i}\pi}{4}-\frac{\mathrm{i}}{\hbar}\int \mathrm{d}x(2m(E-V(x)))^{1/2}\right)\right\}. \tag{23}$$

This expression (23) is thus identical to the usual WKB wavefunction for one-dimensional systems. This result is of significance in view of the apparently different procedures used in the two semiclassical formalisms; the former is based upon the SPA to the transformation theory of Dirac and the other upon an expansion in orders of $\hbar$ with respect to the differential equation of Schrödinger. Furthermore, it is logical to inquire if the equivalence between the CLSM and WKB methods extends to more general systems. In this respect, it is noted that the WKB formalism shares a common quantum mechanical foundation with the CLSM since Dirac (1927) has already shown that the Schrödinger wave equation is subsumed within the transformation theory as a dynamical principle. This enables us to follow a more general approach (Van Vleck 1928) in the development of the WKB from the transformation theory. In the Schrödinger representation, this involves the expansion of the Hamiltonian $H(Q_i, \partial\mathfrak{F}_{ij}/\partial Q_i)$ in powers of $\hbar$, thus resulting in the following equation:

$$\exp(\mathfrak{F}_{ij}(Q_i, P_j; t)/\mathrm{i}\hbar)A_{ij}(Q_i, P_j : t)\left(H\left(Q_i, \frac{\partial\mathfrak{F}_{ij}}{\partial Q_i}\right)+\frac{\partial\mathfrak{F}_{ij}}{\partial t}\right)$$
$$+\mathrm{i}\hbar\exp(\mathfrak{F}_{ij}(Q_i, P_j; t)/\mathrm{i}\hbar)\left(\left(H'\frac{\partial A_{ij}}{\partial Q_i}+\tfrac{1}{2}A_{ij}\frac{\partial H'}{\partial Q_i}\right)+\frac{\partial A_{ij}}{\partial t}\right)$$
$$+\text{terms in higher powers of } \hbar = 0 \tag{24}$$

where $H' = \partial H/\partial(\partial\mathfrak{F}_{ij}/\partial Q_i)$.

From the zeroth-order term in $\hbar$ the Hamilton–Jacobi equation (Goldstein 1950)

$$H\left(Q_i, \frac{\partial\mathfrak{F}_{ij}}{\partial Q_i}\right)+\frac{\partial\mathfrak{F}_{ij}}{\partial t}=0 \tag{25}$$

is recovered and its solution determines the phase function $\mathfrak{F}_{ij}(Q_i, P_j)$. The recovery of the Hamilton–Jacobi equation from equation (24) establishes the following correspondence relation between the quantum phase function and the classical generating function

$$\mathfrak{F}_{ij}(Q_i, P_j) \xrightarrow{\hbar\to 0} F_{ij}(Q_i, P_j). \tag{26}$$

From the first-order term in $\hbar$ of equation (24), the following general equation for the amplitude function $A_{ij}(Q_i, P_j)$ is obtained:

$$\sum_i\left(H_i'\frac{\partial A_{ij}}{\partial Q_i}+\tfrac{1}{2}A_{ij}\frac{\partial H_i'}{\partial Q_i}\right)+\frac{\partial A_{ij}}{\partial t}=0. \tag{27}$$

By making the substitution (Van Vleck 1928)

$$A_{ij}(Q_i, P_j) = \Delta^{1/2}\Theta\left(Q_i, \frac{\partial \mathfrak{F}_{ij}}{\partial Q_i}\right) \qquad \Delta = \frac{\partial^2 \mathfrak{F}_{ij}}{\partial Q_i \partial P_j}(Q_i, P_j) \tag{28}$$

in a conservative system whereupon

$$\frac{\partial A_{ij}}{\partial t} = 0 \tag{29}$$

the equation (27) for the amplitude function simplifies to

$$\sum_i H'_i \frac{\partial \Theta}{\partial Q_i} = 0. \tag{30}$$

The solution for Θ is a constant given by

$$\Theta\left(Q_i, \frac{\partial \mathfrak{F}_{ij}}{\partial Q_i}\right) = C. \tag{31}$$

The transformation function can then be expressed as

$$\langle Q_i | P_j \rangle = \sum_{\substack{\text{classical} \\ \text{trajectories}}} \left(\frac{\partial^2 F_{ij}(Q_i, P_j)}{\partial Q_i \partial P_j}\right)^{1/2} \exp(\mathrm{i} F_{ij}(Q_i, P_j)/\hbar) \tag{32}$$

which is constructed by the superposition of the contributions due to the classical trajectories generated from the Hamilton–Jacobi equation (25). Based upon these WKB transformation functions, the correspondence relation between the mean value $\langle B(q, p)\rangle$ of a dynamical variable $B(q, p)$ and its classical analogue is obtained as shown by

$$\langle B(q,p)\rangle = \int \langle P_j | Q_i \rangle B\left(Q_i, \mathrm{i}\hbar \frac{\partial}{\partial Q_i}\right) \langle Q_i | P_j \rangle \, \mathrm{d}Q_i$$
$$\rightarrow \int B\left(Q_i, \frac{\partial F_{ij}}{\partial Q_i}\right)\left(\frac{\partial^2 F_{ij}}{\partial Q_i \partial P_j}\right) \mathrm{d}Q_i. \tag{33}$$

Thus the correspondence relations and transformation functions of the WKB in a more generalized case are completely identical with similar results of the CLSM. This study has thus shown the complete identity between the WKB and CLSM formalisms for general systems described by the transformation function $\langle Q_i | P_j \rangle$.

3. Discussion and conclusion

This study has traced the development of the WKB and CLSM formalisms from Dirac's transformation theory as the common quantum mechanical foundation to both formalisms. Crucial to this is the ansatz of the transformation function in the form of equation (2) which on the application of the SPA transforms into classical generating functional forms. The adoption of the stationary phase approximation in the CLSM formalism is thus shown to be equivalent to the asymptotic $\hbar$-expansion of the Hamiltonian procedure in the WKB. This conclusion is supported by the complete agreement between the results of the WKB and the CLSM for the transformation functions and the various correspondence relations. Hence, the CLSM and WKB are two different approaches which consistently incorporated the classical limit condition $\hbar \rightarrow 0$ into the transformation theory thereby reducing it to two equivalent semiclassical formalisms with the same level of accuracy.

Having established the equivalence between the WKB and CLSM, this paper thus provides the basis for intermixing the procedures and concepts from both the WKB and CLSM into the semiclassical DWBA for the study of complex nuclear reactions as developed by Hasan and Brink (1978) and later extended into a completely analytical formulation by Wong *et al* (1988) and Wong and Low (1989, 1990). A paper clarifying the relationship of the semiclassical DWBA with the WKB and CLSM is in preparation.

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