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QUASI-CLASSICAL PATH INTEGRALS

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Synopsis.

Various time-independent and time-dependent expansions for non-relativistic motion are considered with a "semi-classical" zero order term. The expansions are expressed with the help of quasi-classical paths. They are all easily combined with a Born expansion. The connection with the BWK method and with the Feynman path integrals is pointed out.

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1. Introduction.

Quasi-classical path integrals occur in various ways in quantum mechanics. Their purpose may range from an expression of a hidden pining for the good old classical theory to a practical tool in an approximation process. Two characteristic forms are the time-independent integrals of, e. g., the BWK approximation[1] and the time-dependent Feynman path integrals[2]. The BWK method is usually restricted to essentially 1-dimensional problems. We shall first deal with the question in how far this restriction is essential to the approximation. Meanwhile we may combine BWK approximation and Born approximation. We further discuss the connection between the time-independent and the time-dependent forms (all non-relativistic). Finally, we consider the singular case of quasi-classical propagation, which occurs in weak fields.

2. 1-dimensional stationary Schrödinger waves.

Consider a particle with mass m in a potential

$$V(x) = V_0(x) + V_1(x). \tag{2.01}$$

The part $V_0(x)$ will be involved in a BWK expansion, the part $V_1(x)$ in a Born expansion. One of them may be zero. The eigenfunctions $\psi(x)$ of the time-independent Schrödinger equation

$$\left\{E + \frac{\hbar^2}{2m}\frac{d^2}{dx^2} - V_0(x)\right\}\psi(x) = V_1(x)\ \psi(x) \tag{2.02}$$

with energy eigenvalue E can arbitrarily be split up into

$$\psi(x) = \psi_+(x) + \psi_-(x) \tag{2.03}$$

with

$$\psi_\pm(x) = A_\pm(x)\, e^{\frac{i}{\hbar} S_\pm(x)}\;;\; A_\pm(x) = B_\pm(x)\, A(x), \qquad (2.04)$$

where $A(x)$ is an arbitrary normalization function and

$$S_\pm(x) = \int^x dx'\; p_\pm(x')\,; \qquad (2.05)$$

$$p_\pm(x) = \pm p(x) = \pm\left\{2m(E - V_0(x)\right\}^{1/2}. \qquad (2.06)$$

The splitting (2.03) can be made unique by an auxiliary condition on the B's. If we choose for this

$$\frac{d\left\{B_+(x)\; A(x)/C(x)\right\}}{dx} e^{\frac{i}{\hbar}S_\pm(x)} + \frac{d\left\{B_-(x)\; A(x)/C(x)\right\}}{dx} e^{\frac{i}{\hbar}S_-(x)} = 0, \quad (2.0'$$

with an arbitrary splitting function $C(x)$, insertion into (2.02) gives for the B's the equations

$$\left.\begin{aligned} \pm \frac{dB_\pm(x)}{dx} e^{\frac{i}{\hbar}S_\pm(x)} = \frac{1}{2}\Bigg\{ &\pm\left(2\frac{A'}{A} + \frac{p'}{p}\right) \\ &+ \frac{\hbar}{ip}\left(\left(\frac{C'}{C}\right)^2 + \left(\frac{C'}{C}\right)'\right) + \frac{2\,mi}{\hbar^2}\, V_1\Bigg\} B_\pm\, e^{\frac{i}{\hbar}S_\pm} \\ + \frac{1}{2}\Bigg\{ &\pm\left(2\frac{C'}{C} + \frac{p'}{p}\right) \\ &+ \frac{\hbar}{ip}\left(\left(\frac{C'}{C}\right)^2 + \left(\frac{C'}{C}\right)'\right) + \frac{2\,mi}{\hbar^2}\, V_1\Bigg\} B_\mp\, e^{\frac{i}{\hbar}S_\mp}. \end{aligned}\right\} \qquad (2.08)$$

The dashes denote the derivatives with respect to x.

We consider such cases for which the coefficients in the right-hand member can be regarded as small, viz., the V_1 terms according to the Born expansion, the derivative terms according to the BWK expansion. So we expand

$$B_\pm(x) = \sum_{r=0}^{\infty} B_\pm^{(r)}(x), \qquad (2.09)$$

with

$$B_\pm^{(0)}(x) = B_\pm^{(0)} \quad \text{(constant)}; \tag{2.10}$$

$$\left.\begin{aligned} \pm\frac{dB_\pm^{(r+1)}(x)}{dx} e^{\frac{i}{\hbar}S_\pm(x)} &= \frac{1}{2}\left\{\pm\left(2\frac{A'}{A}+\frac{p'}{p}\right)\right. \\ &\left.+\frac{\hbar}{ip}\left(\left(\frac{C'}{C}\right)^2+\left(\frac{C'}{C}\right)'\right)+\frac{2mi}{\hbar^2}V_1\right\} B_\pm^{(r)} e^{\frac{i}{\hbar}S_\pm} \\ &+\frac{1}{2}\left\{\pm\left(2\frac{C'}{C}+\frac{p'}{p}\right)\right. \\ +\frac{\hbar}{ip}\left(\left(\frac{C'}{C}\right)^2+\left(\frac{C'}{C}\right)'\right)+\frac{2mi}{\hbar^2}V_1&\left.\vphantom{\frac{C'}{C}}\right\} B_\mp^{(r)} e^{\frac{i}{\hbar}S_\mp} \quad (r = 0,1,\ldots). \end{aligned}\right\} \tag{2.11}$$

In as far as $\psi_+(x)$ and $\psi_-(x)$ are interpreted as the wave components propagating in the + and — directions, respectively, the first part of the right-hand member of (2.11) describes the transmission, and the second part the reflection. The r'th order approximation then accounts for the r-fold transmissions and reflections. But the arbitrariness of the splitting (2.03) according to the choice of the condition (2.07) and the splitting function $C(x)$ (and also the arbitrariness of the normalization function $A(x)$) should be kept in mind.

Integrating (2.11) we have to care for (i) the singular points ("reflection points"), where $E - V_0(x) = 0$ and (ii) the range of (x). For the moment we restrict ourselves to the simplest case of a 2-sided infinite range $-\infty \leq x \leq \infty$ without singularities ($V_0(x) < E$). Then we have the boundary conditions

$$B_\pm^{(r+1)}(x) \xrightarrow[x\to\mp\infty]{} 0 \qquad (r = 0, 1, \ldots), \tag{2.12}$$

and integration of (2.11) gives

$$\left.\begin{aligned} B_\pm^{(r+1)}(x) = \int_{\mp\infty}^{x} dx' \frac{1}{2}\left[\left\{\left(2\frac{A'}{A}+\frac{p'}{p}\right)\right.\right. \\ \pm\frac{\hbar}{ip}\left(\left(\frac{C'}{C}\right)^2+\left(\frac{C'}{C}\right)'\right)\pm\frac{2mi}{\hbar}V_1\left.\vphantom{\frac{C'}{C}}\right\} B_\pm^{(r)} e^{\frac{i}{\hbar}S_\pm} \end{aligned}\right\} \tag{2.13}$$

$$\left.\begin{aligned} &+\left\{\left(2\frac{C'}{C}+\frac{p'}{p}\right)\pm\frac{\hbar}{ip}\left(\left(\frac{C'}{C}\right)^2\right.\right.\\ &\left.\left.+\left(\frac{C'}{C}\right)'\right)\pm\frac{2\,mi}{\hbar}V_1\right\}B_{\mp}^{(r)}\,e^{\frac{i}{\hbar}S_{\mp}}\Bigg]\,e^{-\frac{i}{\hbar}S_{\pm}}\qquad(r=0,1,\ldots).\end{aligned}\right\}\quad(2.13)$$

This corresponds to the iterative solution of the integral equation for $\psi(x)$

$$\left.\begin{aligned}\psi(x) = \psi^0(x) + \int_{-\infty}^{\infty} dx'\,\frac{1}{2}\Bigg[&\left(\frac{A'}{A}+\frac{C'}{C}+\frac{p'}{p}\right)(\psi_+(x')-\psi_-(x'))\\ &+\left(-\frac{A'}{A}+\frac{C'}{C}\right)\frac{x-x'}{|x-x'|}\psi(x')\\ +\left\{\frac{\hbar}{ip}\left(\left(\frac{C'}{C}\right)^2+\left(\frac{C'}{C}\right)'\right)+\frac{2\,mi}{\hbar^2}V_1\right\}&\psi(x')\Bigg]\frac{A(x)}{A(x')}\,e^{\frac{i}{\hbar}|S_{\pm}(x)-S_{\pm}(x')|}\end{aligned}\right\}\quad(2.14)$$

with

$$\psi^0(x) = \psi_+^0(x)+\psi_-^0(x) = B_+^0\,A(x)\,e^{\frac{i}{\hbar}S_+(x)} + B_-^0\,A(x)\,e^{\frac{i}{\hbar}S_-(x)}.\quad(2.15)$$

As long as the continuous potential $V_0(x)$ is approximated by a step potential, the splitting (2.03) can be regarded as unique in each step interval. The continuous limit then corresponds to the choice $C(x) = 1$ for the splitting function. This representation has been used by various authors[3) 4)]. The BWK part of the "reflection coupling coefficient" in (2.11) is then of 1st order, that of the "transmission coupling coefficient" can be made equal to zero by the choice of $A(x) = p(x)^{-1/2}$ for the normalization function.

The choice of $A(x) = C(x) = p(x)^{-1/2}$ reduces the BWK part of all 1st order coefficients to zero and in general will lead to a more rapid convergence (if at all) of the iteration process.

Up to the order $r = 1$ this last choice corresponds to the genuine B[5)]W[6)]K[7)] approximation[1)]. In higher orders the expansions are different, because the genuine method uses an expansion of S rather than of B.

There are many other modifications of the method (e. g. references 8), 9), 10)).

3. 1-dimensional stationary classical waves.

It is well known that the BWK method is actually very much older than quantum mechanics and that much more initials would be needed to do justice to all inventors. We shortly point out the connection with 1-dimensional stationary classical waves (e. g. electromagnetic waves, sound waves) with wave equations of the type

$$\chi(x) - \frac{Z(x)}{ik(x)} \frac{d\psi(x)}{dx} = 0; \tag{3.01}$$

$$ik(x)\, Z(x)\, \psi(x) - \frac{d\chi(x)}{dx} = 0, \tag{3.02}$$

where $k(x)$ is the wave number and $Z(x)$ the impedance. The method of section 2 now leads to the integral equation

$$\left.\begin{aligned} \psi(x) = \psi^{(0)}(x) + \int_{-\infty}^{\infty} dx' \frac{1}{2}\Bigg[\left(\frac{A'}{A} + \frac{C'}{C} + \frac{Z'}{Z}\right)(\psi_+(x') - \psi_-(x')) \\ + \left(-\frac{A'}{A} + \frac{C'}{C}\right)\frac{x-x'}{|x-x'|}\psi(x') \\ + \frac{1}{Z}\left\{\frac{Z}{ik}\left(\frac{C'}{C}\right)^2 - \frac{Z}{ik}\left(\frac{C'}{C}\right)' - \left(\frac{Z}{ik}\right)'\frac{C'}{C}\right\}\psi(x')\Bigg]\frac{A(x)}{A(x')} e^{i|R_\pm(x) - R_\pm(x')|} \end{aligned}\right\} \tag{3.03}$$

with

$$R_\pm(x) = \pm \int^x dx'\, k(x'). \tag{3.04}$$

The BWK part of section 2 is a special case of the present one with

$$Z(x) = k(x) = \frac{p(x)}{\hbar}; \quad R_\pm(x) = \frac{S_\pm(x)}{\hbar}. \tag{3.05}$$

4. Difficulties with more-dimensional stationary waves.

Now consider an N-dimensional system of particles in a total potential

$$V(x) = V_0(x) + V_1(x), \tag{4.01}$$

where (x) stands for all the coordinates $x_1, x_2, \ldots x_N$, and the splitting is done in the same way as in (2.01). The mass of the particle of which x_i is one of the coordinates is written as m_i. We may also add vector potentials

$$A_i(x) = A_{0i}(x) + A_{1i}(x), \tag{4.02}$$

depending on the set of three coordinates of which x_i is one. From the gauge condition of zero divergence we only need the total condition

$$\sum_{i=1}^{N} \frac{1}{m_i} \frac{\partial A_{0i}(x)}{\partial x_i} = \sum_{i=1}^{N} \frac{1}{m_i} \frac{\partial A_{1i}(x)}{\partial x_i} = 0. \tag{4.03}$$

The time-independent Schrödinger equation is then

$$\left.\begin{aligned} &\left\{E - \sum_i' \frac{1}{2m_i}\left(\frac{\hbar}{i}\frac{\partial}{\partial x_i} - A_{0i}(x)\right)^2 - V_0(x)\right\}\psi(x) \\ &\quad = \left\{-\sum_i' \frac{1}{m_i} A_{1i}(x)\left(\frac{\hbar}{i}\frac{\partial}{\partial x_i} - A_{0i}(x)\right)\right. \\ &\qquad \left. + \sum_i' \frac{1}{2m_i} A_{1i}^2(x) + V_1(x)\right\}\psi(x). \end{aligned}\right\} \tag{4.04}$$

In order to proceed in a similar way as in section 2, one needs a set of solutions $S_{0\Lambda}(x)$, depending on an $(N-1)$-dimensional parameter Λ, of the time-independent classical Hamilton-Jacobi equation

$$E - \sum_i' \frac{1}{2m_i}\left(\frac{\partial S_{0\Lambda}(x)}{\partial x_i} - A_{0i}(x)\right)^2 - V_0(x) = 0 \tag{4.05}$$

for the action function $S_{0\Lambda}(x)$. For a given Λ, the $(N-1)$-dimensional surfaces of constant action can be labelled by a 1-dimensional parameter ξ_Λ

$$S_{0\Lambda}(x) = S_{0\Lambda}(\xi_\Lambda). \tag{4.06}$$

Their orthogonal trajectories are the classical paths. ξ_A can serve as a parameter along these paths. In analogy to (2.03), $\psi(x)$ can be written as

$$\psi(x) = \int dA\, \psi_A(x) \tag{4.07}$$

with

$$\psi_A(x) = A_A(x)\, e^{\frac{i}{\hbar} S_{0A}(\xi_A)}. \tag{4.08}$$

As a first attempt one might try to choose the A's constant on the surfaces of constant action

$$A_A(x) = A_A(\xi_A). \tag{4.09}$$

In this case, one should first investigate whether with (4.09) the expansion (4.07) is always possible. Then one would have to account for the coupling throughout the (x)-space between the waves $\psi_A(x)$ with different A's. But, as surfaces of constant action for different A's in general do not coincide, this coupling could not be described directly in terms of the $A_A(\xi_A)$'s. (In case the classical motion is reversible, the surfaces of reverse solutions A and $-A$ conicide. Besides, an auxiliary condition can be imposed upon all pairs $A_A(\xi_A)$ and $A_{-A}(\xi_{-A})$. But, still, the difficulty concerning the coupling with other A's remains).

Instead of an overall coupling between the $\psi_A(x)$'s with different A's, one could try a local coupling in the point (x) between the $\psi_A(x)$'s along the orthogonal trajectory of the corresponding $S_{0A}(\xi_A)$ (classical path) through (x) with different A's. Then, instead of making the restriction (4.09), one would have to impose other auxiliary conditions upon the A's in such a way that (analogous to section **2**) the coupling equations do not contain their second order derivatives and can be separated with regard to the first order derivatives in the direction of the corresponding path. It seems difficult to choose the auxiliary conditions so that we get rid of the second order derivatives, which may be said to describe "scattering" (cf. section **5**). Instead, we shall consider another choice of auxiliary conditions, by which we get rid of "coupling".

5. More-dimensional stationary treatment.

With this other choice it is possible instead of (4.04) to take a more general N-dimensional Schrödinger equation

$$\left\{E - \boldsymbol{H}_0(x)\right\} \psi(x) = \boldsymbol{H}_1(x)\, \psi(x), \tag{5.01}$$

where in the Hamiltonian operator

$$\boldsymbol{H}(x) = \boldsymbol{H}_0(x) + \boldsymbol{H}_1(x) \tag{5.02}$$

the part $\boldsymbol{H}_1$ will again be involved in the Born expansion.

In order to introduce quasi-classical paths we have to define a quasi-classical N-dimensional Hamiltonian $H_0(p,x)$ corresponding to the hermitian operator $\boldsymbol{H}_0(x)$. We can do this, e. g., by means of WEYL's rule of correspondence[11] between (real) functions $a(p,x)$ and (hermitian) operators $\boldsymbol{a}$, which we put in the form[12]

$$\left.\begin{aligned} \boldsymbol{a} &= \iint d\xi^N d\eta^N e^{\frac{i}{\hbar}\sum_i (\xi_i \boldsymbol{p}_i + \eta_i \boldsymbol{x}_i)} \alpha(\xi,\eta) \longleftrightarrow a(p,x) \\ &= \iint d\xi^N d\eta^N e^{\frac{i}{\hbar}\sum_i (\xi_i p_i + \eta_i x_i)} \alpha(\xi,\eta); \end{aligned}\right\} \tag{5.03}$$

$$\left.\begin{aligned} \alpha(\xi,\eta) &= \frac{1}{\hbar^N}\ \mathrm{Trace}\left(e^{\frac{i}{\hbar}\sum_i (\xi_i \boldsymbol{p}_i + \eta_i \boldsymbol{x}_i)} \boldsymbol{a}\right) \\ &= \frac{1}{\hbar^{2N}} \iint dp'^N dx'^N e^{\frac{-i}{\hbar}\sum_i (\xi_i p'_i + \eta_i x'_i)} a(p',x'). \end{aligned}\right\} \tag{5.04}$$

The operators $(\boldsymbol{p})$ and $(\boldsymbol{x})$ read in x-representation

$$\boldsymbol{p}_i = \frac{\hbar}{i}\frac{\partial}{\partial x_i}; \quad \boldsymbol{x}_i = x_i. \tag{5.05}$$

In practice, $H(p,x)$ defined in this way does not contain $\hbar$. Otherwise, one might (at least in sections 5 and 6) instead of $H(p,x)$ also use

$$H_c(p,x) = \lim_{\hbar \to 0} H(p,x), \tag{5.06}$$

which can directly be obtained from

$$H_c(p, x) = \lim_{\hbar \to 0} e^{-\frac{i}{\hbar}\sum_i p_i x_i} \boldsymbol{H}(x)\, e^{\frac{i}{\hbar}\sum_i p_i x_i}. \tag{5.07}$$

If there were a difference at all between H and H_c, it would be at least of 2nd order in $\hbar$. This also holds for other possible choices of the rules of correspondence.

Owing to the relation

$$\frac{\hbar}{i}\frac{\partial}{\partial x_i} e^{\frac{i}{\hbar}S(x)} A(x) = e^{\frac{i}{\hbar}S(x)}\left(\frac{\partial S}{\partial x_i} + \frac{\hbar}{i}\frac{\partial}{\partial x_i}\right) A(x) \tag{5.08}$$

we have[13)]

$$\left.\begin{aligned} \{E - \boldsymbol{H}_0(x)\}\, e^{\frac{i}{\hbar}(x)} A(x) = e^{\frac{i}{\hbar}S(x)} \left\{\left[E - H_0\left(\frac{\partial S}{\partial x}, x\right)\right]\right. \\ - \left[\sum_i \frac{\partial H_0\left(\frac{\partial S}{\partial x}, x\right)}{\partial \frac{\partial S}{\partial x_i}} \frac{\hbar}{i}\frac{\partial}{\partial x_i} + \sum_i \frac{\hbar}{2i} \frac{\partial^2 H_0\left(\frac{\partial S}{\partial x}, x\right)}{\partial x_i \partial \frac{\partial S}{\partial x_i}}\right] \left. - \boldsymbol{Q}_0(x)\right\} \boldsymbol{A}(x). \end{aligned}\right\} \tag{5.09}$$

The hermitian operator $\boldsymbol{Q}_0(x)$ (or $\boldsymbol{Q}_{c0}(x)$ if H_{c0} is used instead of H_0) is at least of 2nd order in $\hbar$. In case of the ordinary Schrödinger equation (4.04), it is

$$\boldsymbol{Q}_0(x) = \sum_i \frac{\hbar^2}{2 m_i} \frac{\partial^2}{\partial x_i^2}. \tag{5.10}$$

The form (5.09) can be used in various ways. If, e. g., one takes $\boldsymbol{H}_1(x) = 0$ and puts

$$\psi(x) = A(x)\, e^{\frac{i}{\hbar}S(x)} \tag{5.11}$$

with real amplitude andp hase functions $A(x)$ and $S(x)$, then the real and imaginary parts can each be equated to zero. This is done (with a longing for the good old classical theory) in the "pilot wave" theories[14) 15)] for the case (4.04), where $\boldsymbol{Q}_0(x)$, according to (5.10), is real and therefore is taken together with the first square brackets of (5.09).

At present we consider, just as in section **4**, a set of solutions $S_{0A}(x)$ of the time-independent Hamilton-Jacobi equation for the action function $S_{0A}(x)$

$$E - H_0\left(\frac{\partial S_{0A}}{\partial x}, x\right) = 0 \tag{5.12}$$

and the corresponding solution $A_{0A}(x)$ of

$$\left[\sum_i \frac{\partial H_0\left(\frac{\partial S_{0A}}{\partial x}, x\right)}{\partial \frac{\partial S_{0A}}{\partial x_i}} \frac{\partial}{\partial x_i} + \sum_i \frac{1}{2} \frac{\partial^2 H_0\left(\frac{\partial S_{0A}}{\partial x}, x\right)}{\partial x_i \partial \frac{\partial S_{0A}}{\partial x_i}}\right] A_{0A}(x) = 0 \tag{5.13}$$

or

$$\sum_i \frac{\partial}{\partial x_i}\left\{\frac{\partial H_0\left(\frac{\partial S_{0A}}{\partial x}, x\right)}{\partial \frac{\partial S_{0A}}{\partial x_i}} A_{0A}(x)^2\right\} = 0. \tag{5.14}$$

The classical paths are again the orthogonal trajectories of the surfaces of constant action (4.06). (5.14) is the stationary continuity equation for the classical density $A_{0A}(x)^2$ along the paths of the system A in a statistical ensemble. Along each path of the solution A we introduce a parameter s_A, for which

$$ds_A = \sum_i dx_{iA} \frac{\partial H_0\left(\frac{\partial S_{0A}}{\partial x}, x\right)}{\partial \frac{\partial S_{0A}}{\partial x_i}} \Bigg/ \sum_i \left(\frac{\partial H_0\left(\frac{\partial S_{0A}}{\partial x}, x\right)}{\partial \frac{\partial S_{0A}}{\partial x_i}}\right)^2, \tag{5.15}$$

where (dx_A) is an infinitesimal element of the path. Instead of the sums in (5.15) we can also take, say, the i^{th} terms only. Integration of (5.13) along that path of the solution A, which goes to (x) from a point (x'), gives

$$A_{0A}(x) = A_{0A}(x') \exp\left\{-\frac{1}{2}\int_{(x')}^{(x)} ds''_A \sum_i \frac{\partial^2 H_0\left(\frac{\partial S_{0A}}{\partial x''}, x''\right)}{\partial x''_i \frac{\partial S_{0A}}{\partial x''_i}}\right\}. \tag{5.16}$$

(x') and $A_{0\Lambda}(x')$ still have to be suitably determined. In the 1-dimensional case, where there is no divergence of paths, the density simply becomes inversely proportional to the velocity

$$A_0(x) = \text{const.} \left(\frac{\partial H_0\left(\frac{\partial S_0}{\partial x}, x\right)}{\partial \frac{\partial S_0}{\partial x}} \right)^{-\frac{1}{2}}. \tag{5.17}$$

In the representation (4.07), (4.08) we now use the auxiliary conditions on the $A_\Lambda(x)$'s, at least in such a way that the $\psi_\Lambda(x)$'s for various values of Λ separately satisfy (5.01). Writing

$$A_\Lambda(x) = B_\Lambda(x)\, A_{0\Lambda}(x), \tag{5.18}$$

that together with (5.09), (5.12), and (5.13) gives the equation

$$\left.\begin{aligned} &\sum_i \frac{\partial H_0\left(\frac{\partial S_{0\Lambda}}{\partial x}, x\right)}{\partial \frac{\partial S_{0\Lambda}}{\partial x_i}} \frac{\partial}{\partial x_i} B_\Lambda(x) \\ &= \frac{-\frac{i}{\hbar}}{A_{0\Lambda}(x)} \left\{\boldsymbol{Q}_0(x) + \boldsymbol{H}_1(x)\right\}\left\{B_\Lambda(x)\, A_{0\Lambda}(x)\right\}. \end{aligned}\right\} \tag{5.19}$$

We consider again such cases where the operators in the right-hand member can be regarded as effectively small, so that we can make the expansion

$$B_\Lambda(x) = \sum_{r=0}^{\infty} B_\Lambda^{(r)}(x) \tag{5.20}$$

with

$$B_\Lambda^{(0)}(x) = B_\Lambda^0 \quad \text{(constant)} \tag{5.21}$$

and

$$\left.\begin{aligned} &\sum_i \frac{H_0\left(\dfrac{\partial S_{0A}}{\partial x}, x\right)}{\partial \dfrac{\partial S_{0A}}{\partial x_i}} \frac{\partial}{\partial x_i} B_A^{(r+1)}(x) \\ &= \frac{-\dfrac{i}{\hbar}}{A_{0A}(x)} \left\{\boldsymbol{Q}_0(x) + \boldsymbol{H}_1(x)\right\}\left\{B_A^{(r)}(x) A_{0A}(x)\right\} \; (r = 0, 1, \ldots). \end{aligned}\right\} \tag{5.22}$$

These equations might be said to describe the "scattering" of the separate semi-classical waves

$$\psi_A^0(x) = A_{0A}(x)\, e^{\frac{i}{\hbar} S_{0A}(x)} \tag{5.23}$$

due to the "quantum potential" operator $\boldsymbol{Q}_0(x)$ and the "Born potential" operator $\boldsymbol{H}_1(x)$ in a similar loose hazy way as (2.11) was said to describe the coupling between the various (two) semi-classical waves.

Integrating (5.22) we have to take care of (*i*) the occurrence of "reflection and scattering singularities" and (*ii*) the range of the coordinates (x) and the boundary conditions. As to (*i*), singularities may occur not only due to the vanishing of the velocity vector in the left-hand member of (5.22), but also due to the operators $\boldsymbol{Q}_0$ and $\boldsymbol{H}_1$ in the right-hand member, e. g., along the envelopes (caustics) of the classical path for a given A. For the moment we restrict ourselves to the simple cases where they do not occur. As to (*ii*), we assume that the region of (x)-space, in which $\boldsymbol{Q}_0$ and $\boldsymbol{H}_1$ are effectively different from zero, can be enclosed in an $(N-1)$-dimensional surface Σ (which may tend to infinity). Let us denote the points where the classical paths cut this surface with the velocity vector pointing towards the inside direction by (x'). Further we assume that the "incoming wave" $\psi^0(x')$ given on Σ can be represented by

$$\psi^0(x') = \int dA\, \psi_A^0(x') \tag{5.24}$$

with

$$\psi_A^0(x') = B_A^0\, A_{0A}(x')\, e^{\frac{i}{\hbar} S_{0A}(x')} \tag{5.25}$$

and a suitable choice for B_A^0 (e. g. 1) and $A_{0A}(x')$. These choices for (x') and $A_{0A}(x')$ will be used in (5.16).

Now we have for (5.22) the boundary conditions

$$B_A^{(r+1)}(x') = 0 \quad (r = 0, 1, \ldots) \tag{5.26}$$

and (5.22) can be integrated along the classical path of the solution $S_{0A}(x)$ which goes to (x) from the corresponding point (x') on Σ

$$\left.\begin{aligned} B_A^{(r+1)}(x)\, A_{0A}(x) &= \int_{(x')}^{(x)} ds''_A \frac{A_{0A}(x)}{A_{0A}(x'')} \frac{-i}{\hbar} \\ \{\boldsymbol{Q}_0(x'') + \boldsymbol{H}_1(x'')\} &\{B_A^{(r)}(x'')\, A_{0A}(x'')\} \quad (r = 0, 1, \ldots). \end{aligned}\right\} \tag{5.27}$$

This corresponds to the iterative solution of the integral equation for $\psi_A(x)$

$$\left.\begin{aligned} \psi_A(x) &= \psi_A^0(x) + \int_{(x')}^{(x)} ds''_A \frac{A_{0A}(x)}{A_{0A}(x'')} \frac{-i}{\hbar} \\ \{\boldsymbol{Q}_0(x'') + \boldsymbol{H}_1(x'')\} &\left\{ e^{\frac{i}{\hbar}\{S_{0A}(x) - S_{0A}(x'')\}} \psi_A(x'') \right\} \end{aligned}\right\} \tag{5.28}$$

with

$$\psi_A^0(x) = B_A^0\, A_{0A}(x)\, e^{\frac{i}{\hbar} S_{0A}(x)} \tag{5.29}$$

as the semi-classical incoming wave.

The genuine BWK approximation, if extended to more than one dimension in higher orders, would again use an expansion of S rather than of B. The present expansion coincides with it up to the order $r = 1$. It seems that in non-separable more-(3-) dimensional problems it has not been used in higher approximation than $r = 0$ (semi-classical waves)[16].

If, for the left-hand member of (5.01), we take the ordinary form (4.04) with $N \leqslant 3$ for a free particle ($A_{0i}(x) = V_0(x) = 0$), the integrations can be carried out for various sets of free particle solutions $S_{0A}(x)$, which all result in the usual Born expansion.

It goes without saying that besides the treatments discussed so far there are many other possibilities (e. g. ref. 17)).

6. Time-dependent treatment.

The notions of coupling in section 2 and of scattering in section 5 should become somewhat clearer in a time-dependent description. The method of section 2 appears not suited to introduce time dependence in a straightforward way, but the method of section 5 can be made more readily fit for it.

Instead of (5.01) we take the time dependent N-dimensional Schrödinger equation

$$\left\{-\frac{\hbar}{i}\frac{\partial}{\partial t}-\boldsymbol{H}_0(x,t)\right\}\psi(x,t)=\boldsymbol{H}_1(x,t)\;\psi(x,t). \qquad (6.01)$$

The Hamiltonian operators may now also depend on time.

Whereas the stationary problem in general is to find the eigenfunctions (and eigenvalues) of (5.01) with certain boundary conditions, the general time dependent problem is to derive from $\psi(x,t')$ at a given time t' (initial condition) $\psi(x,t)$ at other times t. This connection can be expressed by

$$\psi(x,t)=\int dx'^N K(x,t;x',t')\,\psi(x',t'), \qquad (6.02)$$

where $K(x,t;x',t')$ is determined by

$$\left\{-\frac{\hbar}{i}\frac{\partial}{\partial t}-\boldsymbol{H}_0(x,t)\right\}K(x,t;x',t')=\boldsymbol{H}_1(x,t)\,K(x,t;x',t') \quad (6.03)$$

with the initial condition

$$\lim_{t-t'\to 0} K(x,t;x',t')=\delta^N(x-x') \qquad (6.04)$$

and (if (6.03) is understood to be valid for all $t-t'$) a somewhat different representation[18] is obtained if $K(x,t,x',t')$ is multiplied by a factor $\varepsilon(t-t')$, which is 1 for $t>t'$ and 0 for $t<t'$) the inversion condition

$$K(x,t;x',t')=K^*(x',t';x,t). \qquad (6.05)$$

The asterisk denotes the complex conjugate.

In order to introduce quasi-classical paths, we define $H(p,x;t)$ in the same way as $H(p,x)$ in section **5**. Instead of (5.09) we now have

$$\left.\begin{aligned}&\left\{-\frac{\hbar}{i}\frac{\partial}{\partial t}-\boldsymbol{H}_0(x,t)\right\}e^{\frac{i}{\hbar}I(x,t;x',t')}D(x,t;x',t')\\&\quad=e^{\frac{i}{\hbar}I(x,t;x',t')}\left\{\left[\frac{\partial I}{\partial t}-H_0\left(\frac{\partial I}{\partial x},x;t\right)\right]\right.\\&\qquad-\left[\frac{\hbar}{i}\frac{\partial}{\partial t}+\sum_i\frac{\partial H_0\left(\frac{\partial I}{\partial x},x;t\right)}{\partial\frac{\partial I}{\partial x_i}}\frac{\hbar}{i}\frac{\partial}{\partial x_i}\right.\\&+\left.\left.\sum_i\frac{\hbar}{2i}\frac{\partial^2 H_0\left(\frac{\partial I}{\partial x},x;t\right)}{\partial x_i\,\partial\frac{\partial I}{\partial x_i}}\right]-\boldsymbol{Q}_0(x,t)\right\}D(x,t;x',t').\end{aligned}\right\}\quad(6.06)$$

The remarks in section **5**, regarding $\boldsymbol{Q}_0(x)$, also hold for the present $\boldsymbol{Q}_0(x,t)$.

Proceeding in an analogous way as in section **5**, we consider the solutions $I_{0\lambda}(x,t;x',t')$ of the time-dependent Hamilton-Jacobi equation for the principle function ("eikonal") $I_0(x,t;x',t')$ with $t>t'$

$$\frac{\partial I_{0\lambda}(x,t;x',t')}{\partial t}-H_0\left(\frac{\partial I_{0\lambda}(x,t;x',t')}{\partial x},x;t\right)=0\quad(6.07)$$

and the corresponding solutions $D_{0\lambda}(x,t;x',t')$ also with $t>t'$) of

$$\left.\begin{aligned}&\left[\frac{\partial}{\partial t}+\sum_i\frac{\partial H_0\left(\frac{\partial I_{0\lambda}}{\partial x},x;t\right)}{\partial\frac{\partial I_{0\lambda}}{\partial x_i}}\frac{\partial}{\partial x_i}\right.\\&+\left.\sum_i\frac{1}{2}\frac{\partial^2 H_0\left(\frac{\partial I_0}{dx},x;t\right)}{\partial x_i\,\partial\frac{\partial I_0}{\partial x_i}}\right]D_{0\lambda}(x,t;x',t')=0\end{aligned}\right\}\quad(6.08)$$

or

$$\left.\begin{aligned}&\frac{\partial}{\partial t}D_{0\lambda}(x,t;x',t')^2\\&+\sum_i\frac{\partial}{\partial x_i}\left\{\frac{\partial H_0\left(\frac{\partial I_{0\lambda}}{\partial x},x;t\right)}{\partial\frac{\partial I_{0\lambda}}{\partial x_i}}D_{0\lambda}(x,t;x',t')^2\right\}=0.\end{aligned}\right\}\quad(6.09)$$

If there are different solutions $I_{0\lambda}(x,t;x',t')$ (distinguished by hte suffix λ), they correspond to different classical paths from (x') at a time t' to (x) at a time t[19]. Analogous to (5.14), (6.09) is the dynamical continuity equation for the classical density function $D_{0\lambda}(x,t;x',t')^2$. But, whereas (5.14) refers to the paths of the system Λ (all with the same energy E), (6.09) refers to the paths λ starting from (x') at a time t'. This common starting point of diverging paths (which occasionally may also occur in (5.14)*) gives rise to a singularity for $t-t'\to 0$. For the direct (almost straight) classical path from (x') to (x) during the infinitesimal time interval from t' to t we have in (6.08), (6.09)

* Professor A. Bohr informs me about a time-independent 3-dimensional treatment initiated by Christy[32]) and generalized by Fröman[33]), in which one chooses a special system Λ of paths which start from points (x') on a surface Σ (which now may also be inside the region where $\boldsymbol{Q}_0$ and $\boldsymbol{H}_1$ are effective) and converge towards a point (x). For this system Λ, the treatment of section **5** becomes more analogous to that of section **6**. Instead of $S_\Lambda(x)$ and $A_\Lambda(x)$ we may then write $S_\Lambda(x,x')$ and $A_\Lambda(x,x')$. Analogous to (6.10) one has for $(x')\to(x)$ the singularity

$$\lim_{(x')\to(x)}\sum_i\frac{\partial}{\partial x_i'}\frac{\partial H_0\left(\frac{\partial S_0}{\partial x},x'\right)}{\partial\frac{\partial S_0}{\partial x_i'}}=\left\{\sum_i\left(\frac{\partial H_0\left(\frac{\partial S_0}{\partial x},x\right)}{\partial\frac{\partial S_0}{\partial x_i}}\right)^2\right\}^{1/2}\lim_{(x')\to(x)}\frac{N-1}{\left|\vec{x}'-\vec{x}\right|}.\qquad(i)$$

Then

$$J(x,x')=A_\Lambda(x,x')\,e^{\frac{i}{\hbar}S_{0\Lambda}(x,x')}\qquad(ii)$$

is a special solution of (5.01) (in the special form (4.04) with $N=3$; $A_{0i}(x)=0$, with the singularity

$$\lim_{(x')\to(x)}J(x,x')=\lim_{(x')\to(x)}A_{0\Lambda}(x,x')=\lim_{(x')\to(x)}\frac{1}{\left|\vec{x}'-\vec{x}\right|}.\qquad(iii)$$

A general solution $\psi(x)$ is then in Fröman's method with the help of Green's formula expressed as

$$\left.\begin{aligned}&\lim_{t-t'\to 0}\sum_i{}' \left\{\frac{\partial}{\partial x_i}\frac{\partial H_0\left(\frac{\partial I_{0\lambda_0}}{x}, x; t\right)}{\partial\frac{\partial I_{0\lambda_0}}{\partial x_i}}\right\}\\ &= \lim_{t-t'\to 0}\sum_i{}' \left\{\frac{\partial}{\partial x_i}\frac{x_i - x_i'}{t-t'}\right\} = \lim_{t-t'\to 0}\frac{N}{t-t'}.\end{aligned}\right\} \quad (6.10)$$

For the parameter s_λ along the path introduced in analogy to (5.15) we can now take the time t. (6.08) could formally be integrated along the path λ from (x', t') to (x, t)

$$\left.\begin{aligned}&D_{0\lambda}(x, t; x', t') = D_{0\lambda}(x', t'; x', t')\\ &\exp\left\{-\frac{1}{2}\int_{(x',t')}^{(x,t)} dt_\lambda'' \sum_i{}' \frac{\partial^2 H_0\left(\frac{\partial I_{0\lambda}}{\partial x}, x''; t''\right)}{\partial x_i''\,\partial\frac{\partial I_{0\lambda}}{\partial x_i''}}\right\}\end{aligned}\right\} \quad (6.11)$$

similar to (5.16). The singular function $D_{0\lambda}(x',t';x',t')$ is left undetermined. For a classical path λ_0, which for an infinitesimal time interval $t-t'$ is a direct (almost straight) path, the limit

$$\lim_{t-t'\to 0} D_{0\lambda_0}(x, t; x', t')\,(t-t')^{\frac{N}{2}} \quad (6.12)$$

remains finite. If $L\left(x, \frac{dx}{dt}; t\right)$ is a 2nd order polynomial in $\left(\frac{dx}{dt}\right)$, then $D_{0\lambda}^2$ is explicitly given by van Hove's solution[20] (cf. also ref, 16)) of (6.09)

$$D_{0\lambda}(x, t; x', t')^2 = c_\lambda\left\|\frac{\partial^2 I_{0\lambda}(x, t; x', t')}{\partial x_i\,\partial x_j'}\right\|. \quad (6.13)$$

$$\psi(x) = -\frac{1}{4\pi}\int_\Sigma d\Sigma'\left\{\frac{\partial J(x, x')}{\partial x_n}\psi(x') - J(x, x')\frac{\partial\psi(x')}{\partial x_n}\right\}, \quad (iv)$$

where n denotes the direction of the normal on Σ towards (x). This expression (which is analogous to that of Kirchhoff in optics; cf. also ref. 16)), has been used with the semi-classical approximation $J^{(0)}$ for J.

The double bar denotes the determinant of the square matrix $(i, j = 1, 2, \ldots N)$. For more general functions $L\left(x, \frac{dx}{dt}; t\right)$, (6.13) still satisfies (6.09), as can directly be checked with the help of (6.07). Contrary to (6.11), (6.13) fixes the limit for $t - t' \to 0$. As long as the determinant becomes nowhere zero, the constant c_λ can be chosen so that (6.13) is positive. Otherwise, the singularities of $D_{0\lambda}$ have to be carefully investigated. It may be observed that a representation of the solution of (5.14) in terms of $S_{0\lambda}$ analogous to the solution (6.13) of (6.09) in terms of $I_{0\lambda}$ cannot be given.

As the principal function $I_{0\lambda}(x, t; x', t')$ is equal to the path integral of the Langrangian $L_0\left(x, \frac{dx}{dt}; t\right)$

$$I_{0\lambda}(x, t; x', t') = \int_{(x', t')}^{(x, t)} dt''_\lambda L_0\left(x'', \frac{dx''}{dt''}; t''\right), \tag{6.14}$$

the (singular) initial condition for $t - t' \to 0$ for the direct (almost straight) path λ_0 from (x') to (x) during the infinitesimal time interval from t' to t is

$$\lim_{t-t'\to 0} I_{0\lambda_0}(x, t; x', t') = \lim_{t-t'\to 0} (t-t')\, L_0\left(x^v, \frac{x-x'}{t-t}; t\right), \tag{6.15}$$

where (x^v) lies between (x') and (x). The corresponding singularity of (6.13) is then given by

$$\left.\begin{aligned}\lim_{t-t'\to 0} D_{0\lambda_0}(x, t; x', t')^2 = c_{\lambda_0} \lim_{t-t'\to 0} \Bigg\| \Bigg\{ (t-t') \frac{\partial^2}{\partial x_i \partial x_j} \\ + \frac{\partial^2}{\partial x_i \partial\left(\frac{x_j - x_j'}{t-t'}\right)} - \frac{\partial^2}{\partial\left(\frac{x_i - x_i'}{t-t'}\right)\partial x_j} - \frac{1}{t-t'} \\ \frac{\partial^2}{\partial\left(\frac{x_i - x_i'}{t-t'}\right)\partial\left(\frac{x_j - x_j'}{t-t'}\right)}\Bigg\} L_0\left(x^v, \frac{x-x'}{t-t'}; t\right)\Bigg\|\end{aligned}\right\} \tag{6.16}$$

in agreement with (6.12).

If, for $t < t'$, we define

$$I_{0\lambda}(x, t; x', t') = -I_{0\lambda}^{*}(x', t'; x, t) \tag{6.17}$$

(with the asterisk for the case it might become complex) and

$$D_{0\lambda}(x, t; x', t') = D_{0\lambda}^{*}(x', t'; x, t), \tag{6.18}$$

then, for $t < t'$, $I_{0\lambda}(x,t;x',t')$ and $D_{0\lambda}(x,t;x',t')$ in the equations (6.07) — (6.13) have to be replaced by $-I_{0\lambda}^{*}(x, t; x', t')$ and $D_{0\lambda}^{*}(x,t;x',t')$, $\partial/\partial t$ and $\partial/\partial x_i$ by $\partial/\partial t'$ and $\partial/\partial x_i'$, c_λ by $-c_\lambda$. (If the classical motion is reversible, the restrictions of the equations to either $t > t'$ or $t < t'$ can be dropped).

In order to proceed along similar lines as in section **5**, we might (summing over all classical paths from (x') at t' to (x) at t) try to put

$$K(x, t; x', t') = \sum_{\lambda} K_\lambda(x, t; x', t') \tag{6.19}$$

with

$$K_\lambda(x, t; x', t') = D_\lambda(x, t; x', t')\, e^{\frac{i}{\hbar} I_{0\lambda}(x,t;x',t')} \tag{6.20}$$

and make an expansion

$$D_\lambda(x, t; x', t') = \sum_{r=0}^{n} B_\lambda^{(r)}(x, t; x', t')\, D_{0\lambda}(x, t; x', t') \tag{6.21}$$

with

$$B_\lambda^{(0)}(x, t; x', t') = B_\lambda^{0}(x', t'), \tag{6.22}$$

and for $t > t'$

$$\left.\begin{aligned} &\left\{\frac{\partial}{\partial t} + \sum_i \frac{\partial H_0\left(\frac{\partial I_{0\lambda}}{\partial x}, x; t\right)}{\partial \frac{\partial I_{0\lambda}}{\partial x_i}} \frac{\partial}{\partial x_i}\right\} B_\lambda^{(r+1)}(x, t; x', t') \\ &\quad = \frac{-\frac{i}{\hbar}}{D_{0\lambda}(x, t; x', t')} \left\{ \boldsymbol{Q}_0(x, t) + \boldsymbol{H}_1(x, t) \right\} \\ &\qquad \left\{ B_\lambda^{(r)}(x, t; x', t')\, D_{0\lambda}(x, t; x', t') \right\}. \end{aligned}\right\} \tag{6.23}$$

With regard to (6.05) and (6.17), (6.18) we should have for $t < t'$

$$B_\lambda^{(r)}(x, t; x', t') = B_\lambda^{(r)*}(x', t'; x, t). \tag{6.24}$$

Now, if only $I_{0\lambda}$ and $D_{0\lambda}$ would satisfy an initial condition

$$\lim_{t-t'\to 0} \sum_\lambda B_\lambda^0(x', t')\, D_{0\lambda}(x, t; x', t')\, e^{\frac{i}{\hbar} I_{0\lambda}(x, t; x', t')} = \delta^N(x - x') \tag{6.25}$$

for a suitable (perhaps not unique) set of B^0's, we would have for (6.23) the initial conditions

$$\lim_{t-t'\to 0} B_\lambda^{(r+1)}(x, t; x', t') = 0 \quad (r = 0, 1, \ldots). \tag{6.26}$$

If further no „reflection and scattering singulatities'' would occur along the classical paths λ from (x') at t' to (x) at t, then (6.23) could be integrated along these paths

$$\left.\begin{aligned} & B_\lambda^{(r+1)}(x, t; x', t')\, D_{0\lambda}(x, t; x', t') \\ & = \int_{(x', t')}^{(x, t)} dt_\lambda'' \frac{D_{0\lambda}(x, t; x', t')}{D_{0\lambda}(x'', t''; x', t')} \frac{-i}{\hbar} \left\{ \boldsymbol{Q}_0(x'', t'') + \boldsymbol{H}_1(x'', t'') \right\} \\ & \left\{ B_\lambda^{(r)}(x'', t''; x', t')\, D_{0\lambda}(x'', t'', x', t') \right\} \quad (r = 0, 1, \ldots). \end{aligned}\right\} \tag{6.27}$$

This would correspond to the iterative solution of the integral equation for $K_\lambda(x, t; x', t')$

$$\left.\begin{aligned} & K_\lambda(x, t; x', t') = K_\lambda^0(x, t; x', t') \\ & + \int_{(x', t')}^{(x, t)} dt_\lambda'' \frac{D_{0\lambda}(x, t; x', t')}{D_{0\lambda}(x'', t''; x', t')} \frac{-i}{\hbar} \left\{ \boldsymbol{Q}_0(x'', t'') + \boldsymbol{H}_1(x'', t'') \right\} \\ & \left\{ K_\lambda(x'', t''; x'\, t')\, e^{\frac{i}{\hbar} I_{0\lambda}(x, t; x'', t'')} \right\} \end{aligned}\right\} \tag{6.28}$$

with

$$K_\lambda^0(x, t; x', t') = B_\lambda^0(x', t')\, D_{0\lambda}(x, t; x', t')\, e^{\frac{i}{\hbar} I_{0\lambda}(x, t; x', t')} \tag{6.29}$$

as the semi-classical approximation.

If it were only the non-uniqueness of the choice of the $B_\lambda^0(x', t')$ in (6.25), which determines the amplitudes with which the different paths from (x', t') to (x, t) take part in the representation of the propagation process, the problem might be to choose them so as to obtain as good convergence as possible, if convergence is possible at all. The crucial points of the solution are the absence of singularities and the limiting condition (6.25).

For the moment, we restrict ourselves to cases without singularities. It is likely that the occurrence of more than one path λ from (x', t') to (x, t) entails the occurrence of singularities[19]. This would mean that, with our restriction, we have cut off the discussion of such cases.

For the ordinary time-dependent form of the Schrödinger equation (4.04), the limit of the term (6.25) for the direct (almost straight) path from (x') to (x) during the infinitesimal time interval $t - t'$ has been investigated by many authors. It has been done particularly carefully by CHOQUARD[19], who also derived the limits of the other terms for the indirect paths. In fact he finds the latter to be zero, so that our corresponding $B_\lambda^0(x', t')$ in (6.25) would be left indetermined in this case, if it were justified to deal with them at all. The limit for the direct paths actually does give a δ-function in this case. It need not do so for Hamiltonians $H_0(p, x; t)$ which are not 2nd order polynomials in (p). If it does, $B_{\lambda_0}^0(x', t')$ can be determined from

$$\left.\begin{aligned} &\lim_{t-t'\to 0} D_{0\lambda_0}(x, t; x', t')\, e^{\frac{i}{\hbar} I_{0\lambda_0}(x, t; x', t')} \\ = \delta^N(x - x') \lim_{\tau\to 0} \int du^N &\left\{ c_{\lambda_0} \left\| \tau \frac{\partial^2 L^{(as)}(x', u; t)}{\partial u_i \partial u_j} \right\| \right\}^{\frac{1}{2}} e^{\frac{i}{\hbar}\tau L_0^{(as)}(x', u; t)}, \end{aligned}\right\} \quad (6.30)$$

where for $L^{(as)}$ we may take the leading term of L in the asymptotic expression for $\sum_i u_i^2 \to \infty$.

It seems that, just as in section 5, the present expansion has not been used in higher approximations than $r = 0$.

In the present expansion, the "quantum potential" $\boldsymbol{Q}_0$ and the "Born potential" $\boldsymbol{H}_1$ are treated on the same footing. They can also be separated by first taking $K_0(x, t; x', t')$ as the solution of (6.03), (with (6.04), (6.05)) or (6.28) without the terms with $\boldsymbol{H}_1$. Then (cf. [18]), owing to (6.04), $K(x, t; x', t')$ is the solution of the integral equation

$$\left.\begin{aligned}K(x,t;x',t') &= K_0(x,t;x',t')\\ -\frac{i}{\hbar}\int_{t'}^{t} dt'' \int dx''^N\, K_0(x,t;x'',t'')\,\boldsymbol{H}_1(x'',t'')\,&K(x'',t'';x',t').\end{aligned}\right\} \quad (6.31)$$

If $\boldsymbol{H}_1$ is effectively small, (6.31) can again be solved in a Born expansion by iteration.

7. Feynman path integrals.

Another expansion than that of section **6** is used in the Feynman path integrals [2) 20) 21) 22)]. This representation for a time interval from t' to t is obtained by iteration of the (zero order) solution of section **6** for infinitesimal time intervals and then taking the limit (if we were able to do so) of zero time intervals. In this section, we consider the solutions for infinitesimal time intervals from a different point of view than in section **6**, avoiding at the same time the difficulties with possible indirect classical paths.

We use again Weyl's rule of correspondence (5.03), (5.04), from which it follows[12)] that the kernel $a(x,x')$ in x-representation of the operator $\boldsymbol{a}$

$$\boldsymbol{a}\psi(x) = \int dx'^N\, a(x,x')\,\psi(x') \quad (7.01)$$

is connected with the function $a(p,x)$ by

$$a(x,x') = \frac{1}{h^N}\int dp'^N\, e^{\frac{-i}{\hbar}\sum_i (x_i - x_i')\,p_i'}\, a\left(p', \frac{x+x'}{2}\right). \quad (7.02)$$

The solution of (6.03) with (6.04) and (6.05) for an infinitesimal time interval dt is in first order

$$\left.\begin{aligned}K(x,t+dt;x',t) &= \left\{1 - \frac{i}{\hbar}dt\boldsymbol{H}_0(x,t) - \frac{i}{\hbar}dt\boldsymbol{H}_1(x,t)\right\}\delta^N(x-x')\\ &= 1 - \frac{i}{\hbar}dt\,H_0(x,x';t) - \frac{i}{\hbar}dt\,H_1(x,x';t).\end{aligned}\right\} \quad (7.03)$$

The term with H_1 will again be treated as a small perturbation. For the other terms we write, using (7.02),

$$\left.\begin{aligned} &K_0(x, t+dt; x', t) \\ &\quad = \delta^N(x-x') - \frac{i}{\hbar}\, dt\, H_0(x, x'; t) \\ &\quad = \frac{1}{h^N}\int dp'^N\, e^{\frac{i}{\hbar}\sum_i (x_i - x_i')\, p_i'} \left\{1 - \frac{i}{\hbar}\, dt\, H_0\left(p', \frac{x+x'}{2}; t\right)\right\} \\ &\quad \approx \frac{1}{h^N}\int dp'^N\, e^{\frac{i}{\hbar}\left\{\sum_i (x_i - x_i')\, p_i' - dt\, H_0\left(p', \frac{x+x'}{2}; t\right)\right\}}. \end{aligned}\right\} \quad (7.04)$$

In order to obtain the Lagrangian rather than the Hamiltonian, we make, for a suitably chosen (p), the expansion

$$\left.\begin{aligned} &\sum_i \frac{x_i - x_i'}{dt}\, p_i' - H_0\left(p', \frac{x+x'}{2}; t\right) \\ &\quad = \left\{\sum_i \frac{x_i - x_i'}{dt}\, p_i - H_0\left(p, \frac{x+x'}{2}; t\right)\right\} \\ &\quad + \sum_i \left\{\frac{x_i - x_i'}{dt} - \frac{\partial H_0\left(p, \frac{x+x'}{2}; t\right)}{\partial p_i}\right\}(p_i' - p_i) \\ &\quad - \frac{1}{2!}\sum_{i,j} \frac{\partial^2 H_0\left(p, \frac{x+x'}{2}; t\right)}{\partial p_i\, \partial p_j}\, (p_i' - p_i)(p_j' - p_j) \cdot \cdots \end{aligned}\right\} \quad (7.05)$$

Then we could try in (7.04) a stationary phase approximation by choosing (p) so that the first order terms in (7.05) vanish

$$\frac{\partial H_0\left(p, \frac{x+x'}{2}; t\right)}{\partial p_i} = \frac{x_i - x_i'}{dt}. \quad (7.06)$$

For this choice of (p) the zero order terms just give

$$\sum_i \frac{x_i - x_i'}{dt}\, p_i - H_0\left(p, \frac{x+x'}{2}; t\right) = L_0\left(\frac{x+x'}{2}, \frac{x-x'}{dt}; t\right), \quad (7.07)$$

where $L\left(x, \frac{dx}{dt}; t\right)$ is the Lagrangian corresponding to the Hamiltonian $H(p, x; t)$.

The integral (7.04) can now readily be evaluated if the higher than second order terms in (7.05) are zero, i. e. if $H_0(p,x;t)$ is a polynomial in (p) of 2nd order. In this case, we obtain

$$\left.\begin{aligned} K_0(x, t+dt; x', t) = \left(\frac{1}{i\hbar\, dt}\right)^{\frac{N}{2}} \\ \left\| \frac{\partial^2 H_0\left(p, \frac{x+x'}{2}; dt\right)}{\partial p_i\, \partial p_j} \right\|^{-\frac{1}{2}} e^{\frac{i}{\hbar} dt\, L_0\left(\frac{x+x'}{2}, \frac{x-x'}{dt}; t\right)}, \end{aligned}\right\} \quad (7.08)$$

provided the determinant of the second order derivatives of H_0 does not vanish. (Thus, the singular case that $H_0(p,x;t)$ is linear in (p) must be excluded). With the help of (7.06) and the inverse relation

$$\frac{\partial L_0\left(\frac{x+x'}{2}, \frac{x-x'}{dt}; t\right)}{\partial\left(\frac{x_i - x_i'}{dt}\right)} = p_i \quad (7.09)$$

this determinant can (even if H_0 is not a second order polynomial in (p)) be expressed in terms of L_0 by

$$\left.\begin{aligned} \left\| \frac{\partial^2 H_0\left(p, \frac{x+x'}{2}; t\right)}{\partial p_i \partial p_j} \right\|^{-\frac{1}{2}} = \left\{ \frac{\partial(p)}{\partial\left(\frac{x-x'}{dt}\right)} \right\}^{\frac{1}{2}} \\ = \left\| \frac{\partial^2 L_0\left(\frac{x+x'}{2}, \frac{x-x'}{dt}; t\right)}{\partial\left(\frac{x_i - x_i'}{dt}\right) \partial\left(\frac{x_j - x_j'}{dt}\right)} \right\|^{\frac{1}{2}}. \end{aligned}\right\} \quad (7.10)$$

The expression in curled brackets denotes the Jacobian. The resulting

$$\left.\begin{aligned} & K_0(x, t + dt; x', t) \\ & = \left\| \frac{-i}{h\,dt} \frac{\partial^2 L_0\left(\frac{x+x'}{2}, \frac{x-x'}{dt}; t\right)}{\partial\left(\frac{x_i - x_i'}{dt}\right)\partial\left(\frac{x_j - x_j'}{dt}\right)} \right\|^{\frac{1}{2}} e^{\frac{i}{\hbar} dt\, L_0\left(\frac{x+x'}{2}, \frac{x-x'}{dt}; t\right)} \end{aligned}\right\} \quad (7.11)$$

is precisely the zero order contribution (with correct normalization factor) of the direct classical path in section 5 (if also there the correspondence is chosen according to Weyl's rule), in agreement with Choquard's theorem[19] that for infinitesimal time intervals there is no contribution from indirect classical paths.

The case that $H_0(p, x; t)$ is a second order polynomial in (p) is equivalent to the case that $L_0\left(x, \frac{dx}{dt}; t\right)$ is a second order polynomial in $\left(\frac{dx}{dt}\right)$. In other cases, the integral (7.04) will in general not be exactly equal to (7.08) or (7.11) although, according to the principle of stationary phase, the latter expressions might be regarded as more or less appropriate approximations to the first ones—or vice versa.

(7.11) has likewise to satisfy the initial condition (6.04) before it can be regarded as a competitor of (7.04) for giving the most correct description.

If $K_0(x, t; x', t')$ has been found for infinitesimal $t - t'$, it can for finite time intervals formally be obtained by iteration in the well-known way. If $t - t'$ is divided into n infinitesimal intervals $t^{(k+1)} - t^{(k)} = dt^{(k)}$ $(k = 0, 1, \ldots n; (x^{(0)}, t^{(0)}) = (x', t'), (x^{(n+1)}, t^{(n+1)}) = (x, t))$, then

$$\left.\begin{aligned} & K(x, t; x', t') = \lim_{\substack{dt^{(k)} \to 0 \\ (k = 0, 1, \ldots n)}} \prod_{k=0}^{n} \int dx^{(k)^N} \\ & \left\{ K_0(x^{(k+1)}, t^{(k+1)}; x^{(k)}, t^{(k)}) - \frac{i}{\hbar} dt^{(k)} \boldsymbol{H}_1(x^{(k)}, t^{(k)})\, \delta(x^{(k+1)} - x^{(k)}) \right\}. \end{aligned}\right\} \quad (7.12)$$

By lack of an appropriate practical calculus (another formal representation has been given by Davison[22]), this limit can only be treated by approximation methods. Feynman considered it to result from the contributions of all kinematical paths from (x', t')

over $(x^{(1)}, t^{(1)})$, $(x^{(2)}, t^{(2)})$, ... $(x^{(n)}, t^{(n)})$ to (x, t) for all values of $(x^{(1)})$, $(x^{(2)})$, ... $(x^{(n)})$. Because, for infinitesimal $t^{(k+1)} - t^{(k)} = dt^{(k)}$, $K_0(x^{(k+1)}, t^{(k+1)}; x^{(k)}, t^{(k)})$ can in this picture of paths be regarded as due to the direct classical path from $(x^{(k)}, t^{(k)})$ to $(x^{(k+1)}, t^{(k+1)})$, those kinematical paths which, in the limit of all $dt^{(k)} \rightarrow 0$, would not tend to what we vaguely shall call „smooth" paths, will not effectively contribute to (7.12). The criterion when a path is considered to be „smooth" remains to be established.

For the case that (7.11) may be used for K_0 in (7.12), an approximation by stationary phase has been considered by Cécile Morette[20]. The $L_0\left(\frac{x^{(k+1)} + x^{(k)}}{2}, \frac{x^{(k+1)} - x^{(k)}}{dt^{(k)}}; t^{(k)}\right)$'s in the exponents are expanded in powers of the $(x^{(k)} - x_\lambda^{(k)})$'s for suitably chosen $(x_\lambda^{(k)})$'s. In order to make the phase stationary, the first order terms must be made to vanish. They do cancel if the $(x_\lambda^{(k)})$'s are chosen on a classical path λ from (x', t') to (x, t) at the times $t^{(k)}$. Owing to the conditions for infinitesimal time intervals, λ has to be a "smooth" path. The zero order terms, which can be taken before the integral signs in (7.12), then contribute the factor

$$e^{\frac{i}{\hbar}\int_{(x', t')}^{(x, t)} dt''_\lambda \, L_0\left(x'', \frac{dx''}{dt''}; t''\right)} = e^{\frac{i}{\hbar} I_{0\lambda}(x, t; x', t')} . \tag{7.13}$$

If higher than second order terms in the Taylor expansion may be neglected according to the principle of stationary phase, it is seen from comparison with section 6 that, in this approximation, (7.12) is again given by the semi-classical approximation (6.29). Thus, from all the kinematical paths, only the classical path λ yields in the lowest order an effective contribution. It does not seem as if the higher order terms in the present expansion will be less intractable than those in the expansion of section 6. Besides, also here, we come into difficulties if more than one "smooth" classical path is possible from (x', t') to (x, t). The convergence of the Taylor expansion giving a stationary phase near one of them becomes particularly doubtful near the others. One might try to make such an expansion near each of them and hope that contributions from space-time regions far from all of them could be neglected because of phase cancellation, so that (7.12) would split up according to (6.19). In order to determine the amplitudes of the contributions $K_\lambda(x, t; x', t')$ of the various paths, one would even then have to deal with the junctions, with possible singularities along the paths and with possible discontinuities of the paths (or even of their existence) in their dependence on (x, t) and (x', t'). One might hope that (e. g. for fixed (x) and (x') and decreasing $t - t'$) the contributions of paths would turn out to decrease with decreasing "smoothness". Anyhow, these speculations are cut off by the restrictions on the scope of the present paper.

It does not seem that the treatment of the present section could be improved by choosing other rules of correspondence than those of Weyl.

8. Quasi-classical distributions.

In this section, we discuss the particular role of the quasi-classical paths from a somewhat different point of view. To this purpose we use a rather queer and even treacherous representation of quantum mechanics, which (apparently independently and with quite different intentions and interpretations) has been given by a number of authors (cf., e. g., refs. 23), 24), 25), 12)).

To the operators $\boldsymbol{a}$ representing observables and to the statistical operators $\boldsymbol{k}$ representing quantum mixtures[26] we relate functions $a(p, x)$ and $k(p, x)$ in such a way that the expectation value of the observable for the mixture can be written as

$$\text{Trace } (\boldsymbol{k}\,\boldsymbol{a}) = \frac{1}{h^N}\iint dp^N\, dx^N\, h(p, x)\;\; a(p, x). \qquad (8.01)$$

If we relate $a(p, x)$ to $\boldsymbol{a}$ according to Weyl's rule of correspondence (5.03), (5.04), then we have to relate $k(p, x)$ to $\boldsymbol{k}$ in the same way[12]. $k(p, x)$ is then the Wigner distribution[27]. For the special case of a pure quantum state with wave function $\psi(x)$ in the (x)-representation, this becomes

$$k(p, x) = \int d\xi^N\, \psi^\dagger\left(x + \frac{\xi}{2}\right) e^{\frac{i}{\hbar}\sum_i p_i \xi_i}\, \psi\left(x - \frac{\xi}{2}\right). \qquad (8.02)$$

In order to transform the equations of motion, e. g. those in Schrödinger representation

$$\frac{\partial}{\partial t}\boldsymbol{k}(t) = -\frac{i}{\hbar}[\boldsymbol{H}(t), \boldsymbol{k}(t)], \tag{8.03}$$

into the (p, x)-representation, we need the expression which corresponds to the commutator brackets

$$\frac{i}{\hbar}[\boldsymbol{a}, \boldsymbol{b}] = \frac{i}{\hbar}(\boldsymbol{a}\boldsymbol{b} - \boldsymbol{b}\boldsymbol{a}). \tag{8.04}$$

This turns out to be[12)]

$$a(p, x)\frac{2}{\hbar}\left\{\sin\frac{\hbar}{2}\sum_i\left(\frac{6}{6p_i}\frac{\partial}{\partial x_i} - \frac{6}{6x_i}\frac{\partial}{\partial p_i}\right)\right\}b(p, x), \tag{8.05}$$

where the 6 symbol denotes differentiation to the left. The equation of motion for the Wigner quasi-distribution function $k(p, x)$ thus becomes (in Schrödinger representation)

$$\left.\begin{aligned}\frac{\partial}{\partial t}k(p, x; t) &= -H(p, x; t)\\ \frac{2}{\hbar}\sin&\left\{\frac{\hbar}{2}\sum_i\left(\frac{6}{6p_i}\frac{\partial}{\partial x_i} - \frac{6}{6x_i}\frac{\partial}{\partial p_i}\right)\right\}k(p, x; t).\end{aligned}\right\} \tag{8.06}$$

This stochastic equation is only then a point-to-point transformation of the type of classical statistical mechanics

$$\frac{\partial}{\partial t}k_c(p, x; t) = \sum_i\left(\frac{\partial k_c(p, x; t)}{\partial p_i}\frac{dp_i}{dt} + \frac{\partial k_c(p, x; t)}{\partial x_i}\frac{dx_i}{dt}\right), \tag{8.07}$$

if the right-hand member of (8.06) reduces to[12)]

$$-(H(p, x; t),\ k(p, x; t)) \tag{8.08}$$

with the Poisson brackets

$$(a(p, x), b(p, x)) = a(p, x)\left\{\sum_i\left(\frac{6}{6p_i}\frac{\partial}{\partial x_i} - \frac{6}{6x_i}\frac{\partial}{\partial p_i}\right)\right\}b(p, x). \tag{8.09}$$

If we use Heisenberg instead of Schrödinger representation, we obtain a similar condition for the bracket expression of a and H

instead of k and H. The conditions are only satisfied for all operators k and a if $H(p, x; t)$ is a polynomial of 2nd order in (p) and (x).

For the two-sided operators in (8.05) and (8.09) we use the abbreviations

$$\sum_i \left(\frac{6}{6 p_i} \frac{\partial}{\partial x_i} - \frac{6}{6 x_i} \frac{\partial}{\partial p_i} \right) = \mathfrak{P} \tag{8.10}$$

and

$$\frac{2}{\hbar} \sin\left(\frac{\hbar}{2} \mathfrak{P} \right) = \mathfrak{P} + \mathfrak{R}. \tag{8.11}$$

With other rules of correspondence than those used here, $\mathfrak{R}$ may be different. But it is a fundamental feature of correspondence[12)] that, for no linear rule of correspondence, the commutator brackets and the Poisson brackets can correspond to each other identically. Therefore $\mathfrak{R}$ cannot vanish identically. It is of 2nd order in $\hbar$. If $\mathfrak{R}$ and $\boldsymbol{H}_1(p, x; t)$ in

$$H(p, x; t) = H_0(p, x; t) + H_1(p, x; t) \tag{8.12}$$

can be treated as effectively small, we can try the expansion

$$k(p, x; t) = \sum_{r=0}^{\infty} k^{(r)}(p, x; t) \tag{8.13}$$

with

$$\frac{\partial k^{(0)}(p, x; t)}{\partial t} + (H_0(p, x; t), k^{(0)}(p, x; t)) = 0, \tag{8.14}$$

$$\left. \begin{aligned} & \frac{\partial k^{(r+1)}(p, x; t)}{\partial t} + (H_0(p, x; t), k^{(r+1)}(p, x; t)) \\ & = - \left\{ H_0(p, x; t) \mathfrak{R} + H_1(p, x; t) \mathfrak{P} \right\} k^{(r)}(p, x; t) \\ & \qquad (r = 0, 1, \ldots). \end{aligned} \right\} \tag{8.15}$$

According to (8.14), $k^{(0)}(p, x; t)$ varies with time in exactly the same way as a classical distribution function (cf. (8.07)) moves along the classical paths corresponding to the Hamiltonian $H(p, x; t)$. If the classical path, which reaches (p, x) at the time t, starts at the time t' from (p', x'), then

$$k^{(0)}(p, x; t) = k^{(0)}(p', x'; t'). \tag{8.16}$$

Integration of (8.15) along this path gives

$$\left.\begin{array}{c} k^{(r+1)}(p, x; t) = k^{(r+1)}(p', x'; t') \\ -\displaystyle\int_{(p, x'; t')}^{(p, x; t)} dt''_{\lambda} \{ H_0(p'', x''; t'')\,\mathfrak{R} + H_1(p'', x''; t'')\,\mathfrak{P} \} k^{(r)}(p'', x''; t'') \\ (r = 0, 1, \ldots). \end{array}\right\} \tag{8.17}$$

In the present representation there is just one single classical path.

(8.16) and (8.17) correspond to the iterative solution of the integral equation

$$\left.\begin{array}{c} k(p, x; t) = k(p', x'; t') \\ -\displaystyle\int_{(p', x'; t')}^{(p, x; t)} dt''_{\lambda} \{ H_0(p'', x''; t'')\,\mathfrak{R} + H_1(p'', x''; t'')\,\mathfrak{P} \} k(p'', x''; t''). \end{array}\right\} \tag{8.18}$$

The operators $H_0\mathfrak{R}$ and $H_1\mathfrak{P}$ (operating on k) again represent the "quantum scattering" and the "Born scattering". The present equation (8.18) (for the statistical operator $\boldsymbol{k}$) in the variables (p), (x), t, t' more or less corresponds to the equation (6.29) (for the dynamical transformation operator $\boldsymbol{K}(t, t')$) in the variables (x), (x'), t, t', as far as the latter is valid. We shall not try for the moment to transform (8.18) directly from one representation to the other.

The quasi-classical features of the present representation can be seen as an expression of the correspondence principle. The treacherous touch is that it seems to meet to a certain extent that pining for the good old classical theory. It cannot actually do so for various reasons. One of them is the fact that, in any correspondence between quantum operators and quasi-classical functions, the infinitesimal unitary transformations represented by commutator brackets in the quantum representation cannot in general correspond in the same sense to the infinitesimal canonical transformations represented by Poisson brackets in the quasi-classical representation. This leads to „quantum scattering" described by the operator $\mathfrak{R}$. But even in those singular cases (considered in the next section) where this "quantum scattering" is effectively absent, there are still other prohibitive reasons[28) 12)] which fall outside the scope of the present paper.

9. Weak potentials.

If, as in the case of the ordinary Schrödinger equation (4.04), $H_0(p, x; t)$ is a 2nd order polynomial in (p) $\left(\text{and } L_0\left(x, \frac{dx}{dt}; t\right)\right.$ a 2nd order polynomial in $\left.\left(\frac{dx}{dt}\right)\right)$, the limiting condition (6.25) in section **6** and the equivalence of (7.04) and (7.11) in section **7** can be considered as assured. One speaks of a Schrödinger equation with "weak potentials" (or shortly of "weak potentials") if $H_0(p, x; t)$ is a 2nd order polynomial in (p) and (x) $\left(\text{and } L_0\left(x, \frac{dx}{dt}; t\right)\right.$ a 2nd order polynomial in (x) and $\left.\left(\frac{dx}{dt}\right)\right)$. We have seen in section 8 that, in the latter case (and only then), the "quantum scattering" is absent. Then the methods of the preceding sections must also work out rather simply.

In weak potentials there is only one single classical path from (x', t') to (x, t). Difficulties with more than one path do not appear. We may drop the index λ. There is also no ambiguity in $H(p, x; t)$ by the choice of the rules of correspondence.

We shall separate the "Born potential" $\boldsymbol{H}_1$ according to (6.31) and only consider $K_0(x, t; x', t')$.

In weak potentials the expressions

$$\lim_{t-t'\to 0} \frac{\partial^2 I_0(x, t; x', t')}{\partial x_i\, \partial x_j'}, \quad \frac{\partial}{\partial t} \frac{\partial^2 I_0(x, t; x', t')}{\partial x_i\, \partial x_j'} \tag{9.01}$$

are independent of (x), (x') and therefore also

$$\frac{\partial^2 I_0(x, t; x', t')}{\partial x_i\, \partial x_j'}; \; D_0(x, t; x', t')^2. \tag{9.02}$$

If we exclude singularities, the same can be said about $D_0(x, t; x', t')$. Then all successive higher order terms $(r = 0, 1, \ldots)$ of (6.27) (without $\boldsymbol{H}_1$) become zero and (still apart from singularities) the semi-classical expression (6.29) is the exact solution of (6.03), (6.04), (6.05).

The Taylor expansion of L_0 used in section **7** breaks off after the 2nd order terms in the case of weak potentials, and we obtain the same exact solution as according to section 6. So, as is well known, in weak potentials no other Feynman paths yield effective contributions than the one single classical path.

In the representation of section 8 the time dependence of the quasi-distribution $(k(p, x; t)$ in a weak potential is actually described by a point-to-point transformation of the type of classical statistical mechanics (although $k(p, x; t)$ has not the proper type of a classical distribution function).

This case once more illustrates the rather singular behaviour of quantum systems in weak potentials, e. g., the harmonic oscillator[29) 30) 12)]. In particular it shows how dangerous it may be without further investigation to generalize conclusions which have been derived only for the case of weak potentials also to other cases.

10. Conclusion.

The foregoing expansions are just some examples out of a great variety, all with a quasi-classical lowest order term. Even in "weak potentials", where this is the only term, it does not open the gate to the lost classical paradise. For some problems the expansions may be useful as practical approximation methods. In particular the lowest order BWK approximation works in some respects surprisingly well[31)].

As soon as singularities occur, e. g. connected with "classical reflections", the situation near and beyond these points has to be carefully investigated, as it has been done in the stationary 1-dimensional BWK approximation. These singularities are also of importance for the unsolved problem how to deal with various competing classical paths.

A generalization to a relativistic treatment could more readily be performed for the boson than for the fermion case.

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