83. *An Approach to Quasiclassical Approximation for the Schrödinger Equation*

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§1. Introduction. The purpose of the present paper is to show by a certain new approach that there is a geometric- and wave-optical relation, in the literal sense of the word, between the classical mechanics and the quantum mechanics by discussing, as an example and also as an application of our approach, the problem of quasiclassical approximation for the Schrödinger equation. Considerations about the notion of characteristics for the Schrödinger equation lead us to our approach. Our method is to introduce a new real variable s and to look upon the equation in a space of dimension larger than that of the original space by 1 and to apply techniques of the geometric optics to the transformed Schrödinger equation which turns out to be a strongly hyperbolic equation of the second order. Our new variable s has a physical meaning as the action of a motion and leads us to a new formulation of the classical mechanics of particles to which the classical Hamilton-Jacobi theory is reduced.

The present paper is a brief summary of the methods and some results. The proofs and a detailed version of some parts of the present paper will be published in a forthcoming paper.

§2. Transformation of the Schrödinger equation. Let us start with the consideration of Maslov's proposal concerning the notion of characteristics for the Schrödinger equation. Maslov [7] asked of what type the Schrödinger equation is and proposed to take as a characteristic equation for the Schrödinger equation

$$(2\text{–}1)\qquad i\hbar\frac{\partial}{\partial t}\Phi=\frac{1}{2\mu}\sum_{1}^{n}\left(-i\hbar\frac{\partial}{\partial x_j}\right)^2\Phi+V(x,t)\Phi,\ \Phi=\Phi(x,t,\hbar)$$

its corresponding Hamilton-Jacobi equation

$$(2\text{–}2)\qquad \frac{\partial S}{\partial t}+\frac{1}{2\mu}\sum_{1}^{n}\left(\frac{\partial S}{\partial x_j}\right)^2+V(x,t)=0.$$

This equation plays important roles in the W.K.B. expansion for the Schrödinger equation. However, this does not seem to be a natural choice of the characteristic equation of the Schrödinger equation for the following reasons. First, for the Klein-Gordon equation, for example, $\left[\left(i\hbar\frac{\partial}{\partial t}\right)^2-\sum_1^3\left(-i\hbar\frac{\partial}{\partial x_j}\right)^2-\mu^2c^2\right]\Phi=0$, we have two characteristic equations, say, $\left(\frac{\partial S}{\partial t}\right)^2-\sum_1^3\left(\frac{\partial S}{\partial x_j}\right)^2=0$ as in the usual treatment of hyperbolic equations and $\left(\frac{\partial S}{\partial t}\right)^2-\sum_1^3\left(\frac{\partial S}{\partial x_j}\right)^2-\mu^2c^2=0$, according to Maslov, which is the relativistic version of the Hamilton-Jacobi equation for free particles. The second reason, which is essential, is the fact that the characteristic polynomial or the principal symbol of a linear partial differential operator is a polynomial defined on the cotangential projective bundle which is identified with the set of all contact elements of degree 1 of the manifold where the operator is treated. Therefore any characteristic equation must be homogeneous with respect to its cotangential coordinates, which leads us to have a completion of the zeroes of the polynomial $p(x,t,\xi,\tau)=\tau+\frac{1}{2\mu}\sum_1^n\xi_j^2+V(x,t)$ in $T^*(\boldsymbol{R}_x^n\times\boldsymbol{R}_t^1)$ (cotangent bundle over $\boldsymbol{R}_x^n\times\boldsymbol{R}_t^1$). Thus we are led to introduce a new real variable s and embed $T^*(\boldsymbol{R}_x^n\times\boldsymbol{R}_t^1)\times\boldsymbol{R}_s^1$ into $P(T^*(\boldsymbol{R}_x^n\times\boldsymbol{R}_t^1\times\boldsymbol{R}_s^1))$ (cotangential projective bundle over $\boldsymbol{R}_x^n\times\boldsymbol{R}_t^1\times\boldsymbol{R}_s^1$). With any polynomial of degree m, $f=f(\xi_1,\cdots,\xi_n)\in\boldsymbol{C}[\xi_1,\cdots,\xi_n]$ in n indeterminates we associate a new homogeneous polynomial $\hat{f}$ of the same degree in $(n+1)$ indeterminates $\xi_0,\xi_1,\cdots,\xi_n$ by the relation $\hat{f}=\hat{f}(\xi_0,\xi_1,\cdots,\xi_n)=\xi_0^m f(-\xi_0^{-1}\xi_1,\cdots,-\xi_0^{-1}\xi_n)$ and embed the zeroes of f in $\boldsymbol{R}^n$ into the zeroes $(-1,\xi_1,\cdots,\xi_n)$ of $\hat{f}$ in $P^n(\boldsymbol{R})$ (n-dimensional real projective space). For the Hamilton-Jacobi equation (2–2) we take a polynomial $p=p(x,t,\xi,\tau)=\tau+\frac{1}{2\mu}\sum_1^n\xi_j^2+V(x,t)$ defined on $T^*(\boldsymbol{R}_x^n\times\boldsymbol{R}_t^1)$, and by the introduction of a new real variable s and by means of the above mentioned procedure we obtain a homogeneous polynomial $\hat{p}=\hat{p}(x,t,s,\xi,\tau,\sigma)=-\sigma\tau+\frac{1}{2\mu}\sum_1^n\xi_j^2+V(x,t)\sigma^2$ which is defined on $P(T^*(\boldsymbol{R}_x^n\times\boldsymbol{R}_t^1\times\boldsymbol{R}_s^1))$ where σ is the cotangential coordinate for s and is the counterpart of ξ_0 in the procedure of completion mentioned above. This procedure implies for the equation (2–1) to set $\hbar=-\sigma^{-1}$, to multiply the both sides by σ^2 and to transform the unknown by the Fourier transformation $\hat{\psi}(x,t,s)=\frac{1}{2\pi}\int_{-\infty}^{+\infty}e^{is\sigma}\psi(x,t,\sigma)d\sigma$ where we set $\psi(x,t,\sigma)=\Phi(x,t,-\sigma^{-1})$. Now the Schrödinger equation is transformed into the following

$$\text{(2–3)}\quad \hat{P}\hat{\psi}=\left[-\frac{\partial^2}{\partial s\partial t}+\frac{1}{2\mu}\sum_1^n\left(\frac{\partial}{\partial x_j}\right)^2+V(x,t)\frac{\partial^2}{\partial s^2}\right]\hat{\psi}=0,\ \hat{\psi}=\hat{\psi}(x,t,s).$$

As for this operator $\hat{P}$ we have the following

Theorem 1. *The operator $\hat{P}$ is a strongly hyperbolic operator of the second order, and the pseudo-Riemannian metric on $\boldsymbol{R}_x^n \times \boldsymbol{R}_t^1 \times \boldsymbol{R}_s^1$ which admits $\hat{P}$ as its Laplace-Beltrami operator is given by*

$$g = -ds \cdot dt + \frac{\mu}{2} \sum_1^n (dx_j)^2 - V(x, t)(dt)^2.$$

§3. Quasiclassical approximation. The problem of quasiclassical approximation for the initial value problem for the Schrödinger equation

$$i\hbar \frac{\partial}{\partial t}\Phi = \frac{1}{2\mu} \sum_1^n \left(-i\hbar \frac{\partial}{\partial x_j}\right)^2 \Phi + V(x, t)\Phi, \qquad \Phi = \Phi(x, t, \hbar) \tag{3-1}$$

$$\Phi(x, 0, \hbar) = \phi_0(x) \exp\left[\frac{i}{\hbar} S_0(x)\right] \tag{3-2}$$

is transformed to

$$\hat{P}\hat{\psi} = 0, \qquad \hat{\psi} = \hat{\psi}(x, t, s) \tag{3-3}$$

$$\hat{\psi}(x, 0, s) = \phi_0(x)\delta(s - S_0(x)) \tag{3-4}$$

where δ is the Dirac delta-function on the reals with its singularity at the origin. Now we find that *quasiclassical approximation is equivalent to geometric-optical approximation.* Thus the problem is reduced to that of the resolution of singularity of the solution $\hat{\psi}$ and so we seek the solution of the form $\hat{\psi}(x, t, s) = \phi(x, t, s)\delta(s - S(x, t)) + \hat{u}(x, t, s)$ with smooth functions $\hat{u}, \phi, S$ satisfying $\phi(x, 0, s) = \phi_0(x), S(x, 0) = S_0(x)$. Solving this problem and returning to the original (x, t)-space, we have the following

Theorem 2. *We assume that* (i) *$\phi_0(x), S_0(x), V(x, t)$ are real-valued smooth functions,* (ii) *$\phi_0(x)$ is a rapidly decreasing function, and* (iii) *$S_0(x), V(x, t)$ are bounded together with their all derivatives of the first order, and their second and the third derivatives grow at most with the order of polynomials at infinity.*

Then there exists $T > 0$ such that on the time interval $[-T, T]$ the solution of equation (3-1), (3-2) *is decomposed into the form*

$$\Phi(x, t, \hbar) = \phi(x, t, S(x, t)) \exp\left[\frac{i}{\hbar} S(s, t)\right] + \Phi_r(x, t, \hbar)$$

where Φ_r satisfies the following two estimates

$$\sup_{|t| \leqq T} \sup_{\hbar \neq 0} |\hbar|^{-1} \|\Phi_r(x, t, \hbar)\|_{L^2(\boldsymbol{R}_x^n)} < +\infty \tag{1}$$

$$\sup_{|t| \leqq T} \sup_{\hbar \neq 0} |\hbar|^{-1} \left\| -i\hbar \frac{\partial}{\partial x_j} \Phi_r(x, t, \hbar) \right\|_{L^2(\boldsymbol{R}_x^n)} < +\infty \tag{2}$$

and the n-form given by

$$\Omega = \phi(x, t, S(x, t))^2 \left(dx_1 - \frac{1}{\mu} \frac{\partial S}{\partial x_1} dt\right) \wedge \cdots \wedge \left(dx_n - \frac{1}{\mu} \frac{\partial S}{\partial x_n} dt\right)$$

is an invariant form of the vector field $X = \sum_1^n \frac{1}{\mu} \frac{\partial S}{\partial x_j} \frac{\partial}{\partial x_j} + \frac{\partial}{\partial t}$.

Remark 1. The residual term Φ_r is determined by the equation

$$i\hbar\frac{\partial}{\partial t}\Phi_r=\frac{1}{2\mu}\sum_1^n\left(-i\hbar\frac{\partial}{\partial x_j}\right)^2\Phi_r+V(x,t)\Phi_r + \hbar^2\phi_1(x,t,S(x,t))\exp\left[\frac{i}{\hbar}S(x,t)\right] \tag{3–5}$$

$$\Phi_r(x,0,\hbar)=0. \tag{3–6}$$

Here we set $\phi_1(x,t,S(x,t))=(-Y\cdot\phi_2)(x,t,S(x,t))$ where

$$Y=\frac{\partial}{\partial s}-\frac{\partial S}{\partial t}\frac{\partial}{\partial t}-\sum_1^n\frac{\partial S}{\partial x_j}\frac{\partial}{\partial x_j}$$

and

$$\phi_2=-\frac{\partial\phi}{\partial t}+\frac{\partial S}{\partial t}\frac{\partial\phi}{\partial s}-\frac{1}{\mu}\sum_1^n\frac{\partial S}{\partial x_j}\frac{\partial\phi}{\partial x_j}+2V\frac{\partial\phi}{\partial s}-\frac{\phi}{2\mu}\sum_1^n\frac{\partial^2 S}{\partial x_j^2}.$$

Remark 2. The (x,t)-space approach to the latter half of the assertions in Theorem 2 that Ω defines an integral invariant of X has been taken by earlier works. See G. D. Birkoff [1], P. A. Dirac [4], É. Cartan [3]. Our (x,t,s)-space approach together with Cartan's theory of integral invariants will give a more general conservation law.

Remark 3. The pseudo-Riemannian metric in Theorem 1 suggests a possibility of geometric optical reconstruction of the classical mechanics. For a relativistic free particle with mass μ, it suffices to take $g=\mu^2c^2\left\{(cdt)^2-\sum_1^3(dx_j)^2\right\}-(ds)^2$, the corresponding equation of which is the Klein-Gordon equation with roof. Since in a relativistic treatment the cotangential coordinate for the variable s has a physical meaning as (the velocity of light)$\times$(mass), we have to take $g=(cdt)^2-\sum_1^3(dx_j)^2-(ds)^2$, the corresponding operator of which is the 5-dimensional d'Alambertian.

Remark 4. The eikonal equation for $\hat{P}$ is

$$-\frac{\partial\tilde{S}}{\partial s}\frac{\partial\tilde{S}}{\partial t}+\frac{1}{2\mu}\sum\left(\frac{\partial\tilde{S}}{\partial x_j}\right)^2+V(x,t)\left(\frac{\partial\tilde{S}}{\partial s}\right)^2=0.$$

For a phase function of the form $\tilde{S}(x,t,s)=s-S(x,t)$ it reduces to the usual Hamilton-Jacobi equation for $S(x,t)$. In this sense the Hamilton-Jacobi theory of the classical mechanics of particles is a special case of our formulation.

References

[1] Birkoff, G. D.: Some remarks concerning Schrödinger's wave equation. Proc. Nat. Acad. Sci. U. S. A., **39**, 339–344 (1933).

[2] ——: Quantum mechanics and asymptotic series. Bull. Amer. Math. Soc., **39**, 689–700 (1933).

[3] Cartan, É.: Leçons sur les invariants intégraux. Hermann, Paris (1922).

[4] Dirac, P. A. M.: The Principles of Quantum Mechanics (4th edition). Oxford, Claredon Press (1958).

[5] Gårding, L., Kotake, T., et Leray, J.: Problèmes de Cauchy I bis et VI. Bull. Soc. Math. France, **92**, 263–361 (1964).

[6] Leray, J.: Solutions approchées du type de Maslov. Symposium on continuum mechanics and related problems of analysis, Kiev (1971).

[7] Maslov, V. P.: Theory of Perturbation and Asymptotic Methods. M. G. U. (1965).