Appendix A

SEMICLASSICAL APPROXIMATION[1]

Contents

Introduction

In the formulation of Quantum Mechanics that we have seen so far, the central problem is to solve the Schrödinger equation

$$-\frac{\hbar^2}{2m}\nabla^2\Psi\left(\mathbf{r},t\right) + V\left(\mathbf{r},t\right)\Psi\left(\mathbf{r},t\right) = i\hbar\frac{\partial}{\partial t}\Psi\left(\mathbf{r},t\right) \tag{1}$$

under proper conditions, e.g. to have a normalizable wave-function $\Psi\left(\mathbf{r},t\right)$, initial conditions, boundary (or continuity) conditions, etc. Of course there are few cases in which we can solve the differential equation (1) exactly. So people have developed approximation methods. These methods can be divided into *perturbative* ones (based on an expansion in a "small" coupling parameter which may be present in the potential) that will be explored in another course and *non-perturbative* ones. One of these last method will be presented here and it is called *semiclassical* method or *WKB method*, from the name of the three authors G.Wentzel, H.A.Kramers and L.Brillouin who developed it in 1926. The exact reference are G.Wentzel, Zeits f.Physik 38, 518, 1926; H.A.Kramers. Zeits f.Physik 39, 828, 1926; L.Brillouin, Comptes Rendus 183, 24 (1926)).The basic idea is to consider $\hbar$ small. In this case the perturbative coupling of the potential can be any value, even not small. This is the basic reason why this WKB method is called non-perturbative. Another non- perturbative technique which will be explored in later courses is the variational method.

The starting point of the WKB method is the *correspondence principle*. This formal principle tell us that Quantum Mechanical quantities should go into Classical Mechanical ones when $\hbar \to 0$. Actually, as $\hbar$ is a dimension-full quantity, the limit that one should consider is $\hbar/S_{cl} \to 0$, where S_{cl} is the classical action involved in the problem.

This correspondence principle does not mean that Quantum Mechanics (QM) should go exactly into Classical Mechanics (CM) in that limit. In fact we know that in QM there are phases which plays a crucial role and they are not present in CM. What we shall show is that even the QM phases, in that semiclassical limit, can be built using entirely classical "ingredients" (classical trajectories, and Hamilton-Jacobi functions).

We shall in fact see that , by properly re-writing the Schrödinger equation, we can get two coupled equations involving the phase and the modulus of the wave-function. Considering the limit $\hbar \to 0$, we will get that at the zeroth order in $\hbar^2$ the two equations decouples and one of them becomes exactly the *Hamilton-Jacobi* equation. That is the reason why classical "ingredients" derived from this equation can be used in QM in the

semiclassical approximation. Of course the WKB method can go beyond the first order in $\hbar^2$ and we can calculate in principle all corrections to higher orders.

We shall show that, for this approximation to be a good one, not only the ratio $\hbar/S_{cl} \to 0$ must be small but also the variation of the potential in space must be slow.

Chapter 1

The standard WKB method

1.1 Preliminary observations

The wave-function of a physical system is a complex quantity and so it can be written as:

$$\Psi\left(\mathbf{r},t\right) = A\left(\mathbf{r},t\right)\exp\left[\frac{i}{\hbar}S\left(\mathbf{r},t\right)\right], \tag{1.1}$$

where $A\left(\mathbf{r},t\right)$ and $S\left(\mathbf{r},t\right)$ are real functions. Let us insert the expression (1.1) into the Schrödinger equation (1). Next let us first calculate:

$$\nabla^2\Psi\left(\mathbf{r},t\right) = \nabla^2\left\{A\left(\mathbf{r},t\right)\exp\left[\frac{i}{\hbar}S\left(\mathbf{r},t\right)\right]\right\} = \left\{\nabla^2 A\left(\mathbf{r},t\right) + \frac{2i}{\hbar}\boldsymbol{\nabla}A\left(\mathbf{r},t\right)\cdot\boldsymbol{\nabla}S\left(\mathbf{r},t\right) + \right.$$
$$\left. +\frac{i}{\hbar}A\left(\mathbf{r},t\right)\nabla^2 S\left(\mathbf{r},t\right) - \frac{1}{\hbar^2}A\left(\mathbf{r},t\right)\left[\boldsymbol{\nabla}S\left(\mathbf{r},t\right)\right]^2\right\}\exp\left[\frac{i}{\hbar}S\left(\mathbf{r},t\right)\right] \tag{1.2a}$$

and also

$$\frac{\partial}{\partial t}\Psi\left(\mathbf{r},t\right) = \frac{\partial}{\partial t}\left\{A\left(\mathbf{r},t\right)\exp\left[\frac{i}{\hbar}S\left(\mathbf{r},t\right)\right]\right\} = \left\{\frac{\partial}{\partial t}A\left(\mathbf{r},t\right) + \right.$$
$$\left. +\frac{i}{\hbar}A\left(\mathbf{r},t\right)\frac{\partial}{\partial t}S\left(\mathbf{r},t\right)\right\}\exp\left[\frac{i}{\hbar}S\left(\mathbf{r},t\right)\right]. \tag{1.2b}$$

Using (1.2a) and (1.2b), the Schrödinger equation becomes

$$-\frac{\hbar^2}{2m}\nabla^2 A\left(\mathbf{r},t\right) - \frac{i\hbar}{m}\boldsymbol{\nabla}A\left(\mathbf{r},t\right)\cdot\boldsymbol{\nabla}S\left(\mathbf{r},t\right) - \frac{i\hbar}{2m}A\left(\mathbf{r},t\right)\nabla^2 S\left(\mathbf{r},t\right) + $$
$$+\frac{1}{2m}A\left(\mathbf{r},t\right)\left[\boldsymbol{\nabla}S\left(\mathbf{r},t\right)\right]^2 + V\left(\mathbf{r},t\right)A\left(\mathbf{r},t\right) = i\hbar\frac{\partial}{\partial t}A\left(\mathbf{r},t\right) - A\left(\mathbf{r},t\right)\frac{\partial}{\partial t}S\left(\mathbf{r},t\right). \tag{1.3}$$

Equating the real and imaginary part of (1.3) we get the two equations:

$$\frac{\partial}{\partial t}S\left(\mathbf{r},t\right) + \frac{\left[\boldsymbol{\nabla}S\left(\mathbf{r},t\right)\right]^2}{2m} + V\left(\mathbf{r},t\right) = \frac{\hbar^2}{2m}\frac{\nabla^2 A\left(\mathbf{r},t\right)}{A\left(\mathbf{r},t\right)} \tag{1.4a}$$

$$m\frac{\partial}{\partial t}A\left(\mathbf{r},t\right)+\boldsymbol{\nabla}A\left(\mathbf{r},t\right)\cdot\boldsymbol{\nabla}S\left(\mathbf{r},t\right)+\frac{1}{2}A\left(\mathbf{r},t\right)\nabla^2S\left(\mathbf{r},t\right)=0. \tag{1.4b}$$

Note that the second equation represents the *continuity equation* for the probability density. In fact from the definition of probability density we get

$$\wp\equiv\left|\Psi\left(\mathbf{r},t\right)\right|^2=A\left(\mathbf{r},t\right)^2 \tag{1.5}$$

while the probability current density is

$$\mathbf{J}\equiv\mathrm{Re}\left[\Psi^*\left(\mathbf{r},t\right)\frac{\hbar}{im}\boldsymbol{\nabla}\Psi\left(\mathbf{r},t\right)\right]=A\left(\mathbf{r},t\right)^2\frac{\boldsymbol{\nabla}S\left(\mathbf{r},t\right)}{m}, \tag{1.6}$$

So (1.4b) becomes exactly

$$\frac{\partial\wp}{\partial t}+\boldsymbol{\nabla}\cdot\mathbf{J}=0. \tag{1.7}$$

Moreover let us note that eq. (1.4a), if we stop at the zero-th order in $\hbar^2$, becomes the *classical Hamilton-Jacobi equation*[1]

$$\frac{\partial}{\partial t}S_0\left(\mathbf{r},t\right)+\frac{\left[\boldsymbol{\nabla}S_0\left(\mathbf{r},t\right)\right]^2}{2m}+V\left(\mathbf{r},t\right)=0. \tag{1.8}$$

Let us review here, even if we have already seen it before, the principal features of this equation.

1.2 Review of the Hamilton-Jacobi equation

As we have learned in the first part of the course, the equations of the Hamiltonian formulation of CM involve the *canonical variables* $x_1...x_{2f}$, i.e. the configurational variables $q_1...q_f$ and the conjugate momenta $p_1...p_f$, and they have the form [2]

$$\dot{q}_k = \{q_k,H\}_{PB} \tag{1.9a}$$
$$\dot{p}_k = \{p_k,H\}_{PB} \tag{1.9b}$$

with $k=1...f$, for a system with f degrees of freedom and Hamiltonian H. We have also introduced particular transformations among the canonical variables:

$$Q_k = Q_k\left(q_1...q_f,p_1...p_f,t\right) \tag{1.10a}$$
$$P_k = P_k\left(q_1...q_f,p_1...p_f,t\right) \tag{1.10b}$$

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[1] We wrote $S_0\left(\mathbf{r},t\right)$ and not simply $S\left(\mathbf{r},t\right)$ to underline the fact that we work at the zero-th order (with respect to $\hbar^2$).

[2] We have used the Poisson Bracket notations

$$\{F,G\}_{PB}\equiv\sum_{k=1}^{f}\left[\frac{\partial F}{\partial q_k}\frac{\partial G}{\partial p_k}-\frac{\partial F}{\partial p_k}\frac{\partial G}{\partial q_k}\right].$$

which keep invariant the Hamilton equation of motion:such transformations are called *canonical*. We shall indicate with $X_1...X_{2f}$ the new variables of phase-space and with K the new Hamiltonian. For a transformation to be canonical the fundamental condition (called *symplectic condition*) that must be satisfied is

$$\underline{\underline{\mathbf{M}}} \, \underline{\underline{\mathbf{J}}} \, \underline{\underline{\mathbf{M}}}^T = \underline{\underline{\mathbf{J}}} \tag{1.11}$$

where $\underline{\underline{\mathbf{M}}}$ is the Jacobian matrix of the transformation

$$\underline{\underline{\mathbf{M}}} \equiv \frac{\partial \mathbf{X}}{\partial \mathbf{x}} = \frac{\partial \left(\mathbf{Q}, \mathbf{P} \right)}{\partial \left(\mathbf{q}, \mathbf{p} \right)} = \frac{\partial \left(Q_1...Q_f, P_1...P_f \right)}{\partial \left(q_1...q_f, p_1...p_f \right)} \tag{1.12}$$

and $\underline{\underline{\mathbf{J}}}$ is called Poisson Matrix.

$$\underline{\underline{\mathbf{J}}} \equiv \begin{pmatrix} \underline{\underline{\mathbf{0}}}_{f \times f} & \underline{\underline{\mathbf{1}}}_{f \times f} \\ -\underline{\underline{\mathbf{1}}}_{f \times f} & \underline{\underline{\mathbf{0}}}_{f \times f} \end{pmatrix}_{2f \times 2f}. \tag{1.13}$$

We all know that, on the basis of Hamilton variational principle, the solutions of eqs. (1.9a) and (1.9b) satisfy the variational equation

$$\delta \int_{t_1}^{t_2} dt \, \mathcal{L} \left(q_1, ..., q_f, \dot{q}_1, ..., \dot{q}_f, t \right) = \delta \int_{t_1}^{t_2} dt \left[\sum_{k=1}^{f} \dot{q}_k p_k - H \left(q_1, ..., q_f, p_1, ..., p_f, t \right) \right] = 0. \tag{1.14}$$

An analog equation is valid for the new phase-space variables (1.10a) and (1.10b), i.e.

$$\delta \int_{t_1}^{t_2} dt \left[\sum_{k=1}^{f} \dot{Q}_k P_k - K \left(Q_1...Q_f, P_1...P_f \right) \right] = 0. \tag{1.15}$$

The two equations (1.14) and (1.15) describe the same physical system if the symplectic condition (1.11) is satisfied or, equivalently, if the integrands differ by a total derivative of a function [3] $F(\mathbf{q}, \mathbf{P}, t)$. F is called the generating function of the canonical transformation. In fact, from the imposition that 1.14) and (1.15) differ by a total derivative, we get that:

$$\frac{\partial}{\partial q_k} F(\mathbf{q}, \mathbf{P}, t) = p_k \tag{1.16a}$$

$$\frac{\partial}{\partial P_k} F(\mathbf{q}, \mathbf{P}, t) = Q_k \tag{1.16b}$$

$$\frac{\partial}{\partial t} F(\mathbf{q}, \mathbf{P}, t) + H = K. \tag{1.16c}$$

By properly choosing the canonical transformation, it is possible to obtain from (1.16c) a transformation such that $K \left(Q_1...Q_f, P_1...P_f \right) = 0$; the relative equations of motion

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[3]For simplicity we shall use the symbols $\mathbf{q}$ e $\mathbf{p}$ to indicate respectively $q_1...q_f$ and $p_1...p_f$.

for the associated variables tells us that these are constants of motion. A canonical transformation of this type is generated by an $F(\mathbf{q}, \mathbf{P}, t)$ such that, by using (1.16c) and the (1.16a), we get

$$\frac{\partial}{\partial t}F(\mathbf{q}, \mathbf{P}, t) + H(\mathbf{q}, \mathbf{p}, t) = 0 \Rightarrow \frac{\partial}{\partial t}F(\mathbf{q}, \mathbf{P}, t) + H\left(\mathbf{q}, \frac{\partial}{\partial \mathbf{q}}F(\mathbf{q}, \mathbf{P}, t), t\right) = 0. \quad (1.17)$$

This is exactly the Hamilton-Jacobi equation: it is a non-linear partial differential equation for F. Using Hamilton variational methods (with variations also of the time at the extremes), it is possible to prove that the Hamilton-Jacobi equation is satisfied by the classical action *function* (which should not be confused with the action *functional*).

$$F(\mathbf{q}, \mathbf{P}, t) = S_{cl}(\mathbf{q}, \mathbf{P}, t) = \int_{t_1}^{t} dt' \ \mathcal{L}\left(\mathbf{q}_{cl}\left(t'\right), \dot{\mathbf{q}}_{cl}\left(t'\right), t'\right), \quad (1.18)$$

The subindex (cl) indicates that we refer to the action calculated along a trajectory $\mathbf{q}(t)$ which satisfies the classical equations of motion with boundary conditions $\mathbf{q}_{cl}(t_1) = \mathbf{q}_1$ and $\mathbf{p}_{cl}(t_1) = \mathbf{P}$.

Considering for simplicity the motion of a single particle of mass m in a potential $V(\mathbf{r})$, We can write its Lagrangian in Cartesian coordinates as

$$\mathcal{L} = \frac{m}{2}\dot{\mathbf{r}}^2 - V(\mathbf{r}) = \frac{\mathbf{p}^2}{2m} - V(\mathbf{r}), \quad (1.19)$$

then, using eq. (1.16a), we get [4]

$$\mathbf{p} = \frac{\partial \mathcal{L}}{\partial \dot{\mathbf{r}}} = m\dot{\mathbf{r}} = \frac{\partial S_{cl}}{\partial \mathbf{r}} = \boldsymbol{\nabla} S_{cl}. \quad (1.20)$$

Then the Hamilton-Jacobi equation becomes simply

$$\frac{\partial}{\partial t}S_{cl} + \frac{[\boldsymbol{\nabla} S_{cl}]^2}{2m} + V = 0, \quad (1.21)$$

which is the same eq. (1.8) found in1.1.

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[4]Here and in (1.17) we have used the symbol of derivation with respect to a vector with the meaning of gradient with respect to that vector, i.e. a

$$\frac{\partial}{\partial \mathbf{q}} \equiv \boldsymbol{\nabla}_{\mathbf{q}}$$

$$\frac{\partial}{\partial \mathbf{r}} \equiv \boldsymbol{\nabla}_{\mathbf{r}} = \boldsymbol{\nabla}.$$

Actually $\mathbf{q}$ is not a vector in the usual sense that means in the sense of vector with respect to the rotation group in $\mathbb{R}^3$, but it is only an object with n components.

1.3 The WKB method

1.3.1 Generalities

Let us go back to Quantum Mechanics and let us see how we can use the eqs. we found to write down approximate solutions to the Schrödinger equation. Let us make the assumption that the potential changes very slowly as a function of the spatial coordinates. For simplicity we shall work with a 1-dimensional Schrödinger operator whose eigenvalue equation is [5], i.e.

$$\frac{d^2\psi(x)}{dx^2} + \frac{2m}{\hbar^2}[E - V(x)]\psi(x) = 0. \tag{1.22}$$

If $V = const.$ and $E > V$, the eq. (1.22) has solutions of the form $Ae^{\pm ikx}$ with $k \equiv \sqrt{2m(E-V)}/\hbar$, which are waves of amplitudes A and constant wave-length $\lambda = 2\pi/k$. If the potential varies very slowly in x on a scale-length of λ, it is reasonable to suppose that the solutions remain the same but with a slowly varying amplitude and wavelength. Analogously, if $V = const.$ but $E < V$ then eq. (1.22) has solutions of the form $Ae^{\pm\kappa x}$ with $\kappa \equiv \sqrt{2m(V-E)}/\hbar$, i.e. exponentially decaying wave-functions. Again, supposing that the potential changes very slowly with respect to $1/\kappa$, the solution will remain an exponential but with A and κ slowly varying.

It is immediately clear that our considerations will give a reasonable approximation only in particular regions of the domain of ψ (which we will better characterize later on). We should note in fact that in the regions where $E \approx V$, the quantities λ and $1/\kappa$ go to $+\infty$, so it is not reasonable to suppose that $V(x)$ is a slowly varying function on the scale of λ. These critical points are called *turning points* and classically are the points in which the particle changes its direction of motion. The mathematical treatment of the solutions in a neighbor of these points is rather cumbersome and we will let the interested reader study it in more advanced books.

1.3.2 The WKB solutions and their validity

Far from the turning points we can try a solution of the form

$$\psi(x) = \exp\left[\frac{i}{\hbar}u(x)\right], \tag{1.23}$$

where now the function[6] $u(x)$ is not necessarily linear in x as in the cases of constant potential considered before. Actually, we shall go on like in section 1.1, but, with respect to the parametrization used in (1.1), $u(x)$ is now

$$u(x) = S + \frac{\hbar}{i}\ln A; \tag{1.24}$$

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[5] Let us remember that the Schroedinger eq. (1) has solutions of the form

$$\Psi(\mathbf{r}, t) = \psi_E(\mathbf{r}) \exp\left[-\frac{i}{\hbar}E(t - t_0)\right].$$

[6] The function $u(x)$ must be complex.

As before, inserting (1.23) in (1.22)), we shall find two coupled equations which are nothing else that the 1-dimensional analog of eqs. (1.4a) and (1.4b):

$$\left(S'\right)^2 - 2m(E-V) = \hbar^2 \frac{A''}{A} \tag{1.25a}$$

$$2A'S' + AS'' = 0. \tag{1.25b}$$

From (1.25b) by integration we get immediately that:

$$A = \frac{const.}{\left(S'\right)^{1/2}}; \tag{1.26}$$

If we now replace this expression in (1.25a), we get

$$\left(S'\right)^2 = 2m(E-V) + \hbar^2 \left[\frac{3}{4}\left(\frac{S''}{S'}\right)^2 - \frac{1}{2}\frac{S'''}{S'}\right], \tag{1.27}$$

This equation is rigorously equivalent to the Schrödinger equation we started from (1.22). The WKB approximation is basically an expansion of S in powers of $\hbar^2$

$$S = S_0 + \hbar^2 S_1 + ... \tag{1.28}$$

Of course we shall keep only the lowest order terms $\hbar^2$. The reason why the expansion has been done in $\hbar^2$ and not in $\hbar$ is that in (1.27) the $\hbar^2$ makes its appearance and not $\hbar$.

At this point we can rewrite the (1.23) as

$$\psi\left(x\right) = A \exp\left[\frac{i}{\hbar}S\right] = A \exp\left[\frac{i}{\hbar}\left(S_0 + \hbar^2 S_1 + ...\right)\right]. \tag{1.29}$$

Inserting the (1.28) into (1.27) and looking only at the zero-order in $\hbar^2$ we get

$$\left(S_0'\right)^2 = 2m(E-V). \tag{1.30}$$

Using the following definitions

$$\lambda \equiv \frac{1}{k} = \frac{\hbar}{\sqrt{2m(E-V)}}, \text{ per } E > V \tag{1.31a}$$

$$\ell \equiv \frac{1}{\kappa} = \frac{\hbar}{\sqrt{2m(V-E)}}, \text{ per } E < V \tag{1.31b}$$

the equation (1.30) becomes

$$S_0' = \pm\frac{\hbar}{\lambda} = \pm\hbar k, \text{ per } E > V \tag{1.32a}$$

$$S_0' = \pm i\frac{\hbar}{\ell} = \pm i\hbar\kappa, \text{ per } E < V. \tag{1.32b}$$

So the WKB solutions have the form:

$$\psi\left(x\right) \approx A \exp\left[\frac{i}{\hbar}S_0\right], \tag{1.33}$$

which, using (1.26), becomes:

$$\psi\left(x\right) \quad \approx \quad \psi_{WKB}\left(x\right) = \frac{C}{\sqrt{k\left(x\right)}} \exp\left[\pm i \int k\left(x\right) dx\right], \text{ per } E > V \tag{1.34a}$$

$$\psi\left(x\right) \quad \approx \quad \psi_{WKB}\left(x\right) = \frac{C}{\sqrt{\kappa\left(x\right)}} \exp\left[\pm \int \kappa\left(x\right) dx\right], \text{ per } E < V. \tag{1.34b}$$

The general approximate solutions will be linear combinations of the two terms above (with the $+$ and with $-$). It is interesting to observe that, in the classically allowed region (i.e. for $E > V$), we have that

$$\wp \equiv \left|\psi\left(x\right)\right|^2 \approx \frac{\left|C\right|^2}{k\left(x\right)} \propto \frac{1}{p\left(x\right)}; \tag{1.35}$$

This equation shows that the probability to find the particle at the point x is inversely proportional to its linear momentum $p\left(x\right)$, i.e. to its velocity, exactly as in classical mechanics.

When one uses approximation methods, it is always necessary to specify mathematically the limits of applicability of the method. To just say that the WKB works well for slowly varying potential is not a mathematical precise statement. If we want to be more precise, let us note from (1.29) that the corrections of order $\hbar^2$ brings into the WKB solutions only a further phase factor $\exp\left[i\hbar S_1\right]$. This factor can be neglected only if $\hbar S_1 \ll 1$. At this point it is enough to insert the expansion (1.28) in (1.27) and equate the terms of order $\hbar^2$. For example for $E > V$, we find after simple calculations

$$\hbar S_1' = \pm \left[\frac{1}{4}\lambda'' - \frac{1}{8}\frac{\left(\lambda'\right)^2}{\lambda}\right] \Longrightarrow \hbar S_1 = \pm \left[\frac{1}{4}\lambda' - \frac{1}{8}\int \frac{\left(\lambda'\right)^2}{\lambda} dx\right]. \tag{1.36}$$

From these equations, we get that the criterion for the WKB approximation is

$$\lambda'\left(x\right) \quad \ll \quad 1, \text{ for } E > V \tag{1.37a}$$

$$\ell'\left(x\right) \quad \ll \quad 1, \text{ for } E < V \tag{1.37b}$$

If we make explicit the dependence from the potential we get the validity condition:

$$\frac{\left|m\hbar V'\left(x\right)\right|}{\left|2m\left[E - V\left(x\right)\right]\right|^{3/2}} \ll 1. \tag{1.38}$$

This equation is a more mathematically precise characterization of the statement that the potential must be slowly varying with x.

1.3.3 Connecting formulas

When $E = V$ the quantities previously defined, i.e. λ and ℓ, diverge and the approximations used are not valid anymore. In fact note that the LHS of (1.38) diverges at the turning points (if $V'(x)$ is finite). Let us suppose that $E \lessgtr V$ for $x \lessgtr a$. If the WKB approximation can be used everywhere except in a neighbor of the turning point $x = a$, we have that

$$\psi_{WKB}(x) = \frac{A}{\sqrt{\kappa(x)}} \exp\left[-\int_a^x \kappa(x)\,dx\right] + \frac{B}{\sqrt{\kappa(x)}} \exp\left[+\int_a^x \kappa(x)\,dx\right],\ \text{for } x < a$$

$$(1.39)$$

and

$$\psi_{WKB}(x) = \frac{C}{\sqrt{k(x)}} \exp\left[-i\int_a^x k(x)\,dx\right] + \frac{D}{\sqrt{k(x)}} \exp\left[+i\int_a^x k(x)\,dx\right],\ \text{for } x > a.$$

$$(1.40)$$

The problem now is to find out how the coefficients C and D can be related to A and B. If we manage to do that, we can bypass the problem of finding the exact WKB solution in the neighbor of the turning points where the WKB solution fails. We will only report here the "connecting formulas" which connects the "oscillating WKB solutions" to the "exponentially decaying solutions" and let the interested reader study its derivation in more advanced books

$$\frac{A}{\sqrt{\kappa(x)}} \exp\left[-\int_x^a \kappa(x)\,dx\right] + \frac{B}{\sqrt{\kappa(x)}} \exp\left[+\int_x^a \kappa(x)\,dx\right] \longleftrightarrow$$

$$\longleftrightarrow \frac{2A}{\sqrt{k(x)}} \cos\left[\int_a^x k(x)\,dx - \frac{\pi}{4}\right] - \frac{B}{\sqrt{k(x)}} \sin\left[\int_a^x k(x)\,dx - \frac{\pi}{4}\right] \quad (1.41)$$

Clearly the oscillating solutions are valid in $x \ll a$, while the exponential ones are valid in $x \gg a$. Analogous formulas are valid in the case in which $V \lessgtr E$ for $x \lessgtr a$.

1.3.4 The "analogy" between Wave-optics versus Geometrical optics and Quantum Mechanics versus Classical Mechanics

To conclude this brief exposition of the WKB we would like to draw the attention of the reader to the analogy indicated in the title of this section.

In optics the student has for sure studied all the phenomena related to wave optics like interference, diffraction and similar. They are all phenomenon based on the wave nature of light. In all these phenomenon the wavelength of light has dimension comparable with the system with which it interacts. Geometrical optics instead is an approximation to wave optics which is valid in the cases in which the wavelength is much smaller than the system with which light interacts. In geometrical optics rays (and not waves) are the central objects together with their trajectories (through lenses and other big devices).

Quantum Mechanics which gives a wave nature to particles is the "analog" of Wave optics and it has to be used in those cases in which the wavelength of the particles is

comparable with the systems with which it interacts, typically atoms. Doing the WKB approximation we have studied that regime of QM in which $\hbar$ is small or equivalently the wavelength of the particle is small compared to the variation of the potential. We have also seen that all elements of the WKB can be prepared with "ingredients" coming from CM. So the WKB or, even better, CM is like the geometrical optics associated to QM. In CM we have rays that are the classical trajectories but we have also the analog of wave-fronts which are the $S(q)$ functions solutions of the Hamilton-Jacobi equations.

Another analogy between "geometrical optics" and classical mechanics is the following: the Huygens principle of geometrical optics says that the rays run along trajectories of minimum optical paths and this is the analog of the Hamilton variational principle which says that the classical trajectories are those which minimize the action.

Of course the analogy, especially between QM and wave-optic, should be taken with some caution. In fact while in optics the effects of interference and so on takes places between quantities (the field strength) that we measure, in QM the interference is among wave-functions that we do not directly measure. Nevertheless the physical effects of the wave-nature of the wave-functions manifest themselves as we all know.

1.4 An application of the WKB: α particles emission from the nucleus

We shall now apply the WKB method to the calculation of the transmission coefficient through the potential barrier represented in the figure 1.1. This calculation is useful for the α decay of the nuclei.
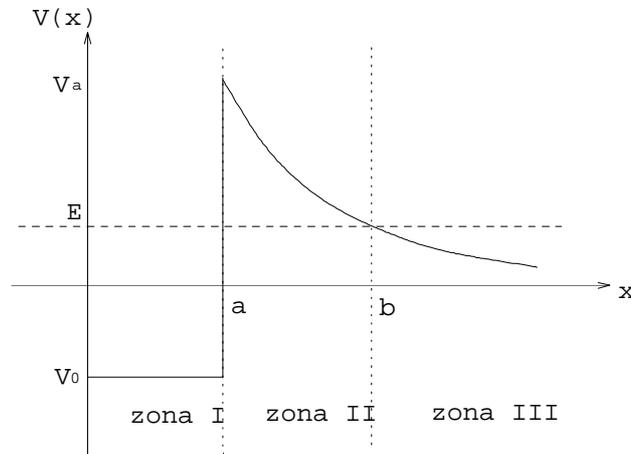
Figure 1.1: Model of the potential barrier in the α decay of the nuclei.

A nucleus (of ray a and charge Z) is roughly represented by a potential well of depth V_0. For $x > a$, the potential is of the Coulomb type and goes to zero for $x \to \infty$. Let us

suppose that inside the nucleus there is a small bunch of matter ($\alpha-$particle with charge z) and energy $E > 0$. Let us indicate with $x = b$ the point in which

$$\frac{zZe^2}{4\pi\varepsilon_0 b} = E. \tag{1.42}$$

Let us now look at the problem. We have to build a solution of the Schrödinger equation which in the zone III behaves as a wave (transmitted wave) . In that region, using the WKB approximation developed previously and the standard notation, the solution has the form

$$\psi_{III}(x) \sim \frac{C}{\sqrt{k(x)}} \exp\left[\pm i \int k(x)\, dx\right]. \tag{1.43}$$

To simplify the calculations , let us choose waves which propagates in the direction of positive x. Let us insert a phase of $\pi/4$ and we get

$$\psi_{III}(x) = \frac{1}{\sqrt{k(x)}} \exp\left[i \int_b^x k(x')\, dx' + i\frac{\pi}{4}\right] =$$
$$= \frac{1}{\sqrt{k(x)}} \left[\cos\left(\int_b^x k(x')\, dx' + \frac{\pi}{4}\right) + i\sin\left(\int_b^x k(x')\, dx' + \frac{\pi}{4}\right)\right]. \tag{1.44}$$

We have now to make use of the connecting formulas in order to extend the solution to the zone II. Extending only the sin function (because the cos function would give an increasing exponential), we have that

$$\psi_{II}(x) = \frac{-i}{\sqrt{\kappa(x)}} \exp\left[\int_x^b \kappa(x')\, dx'\right] =$$
$$= \frac{-i}{\sqrt{\kappa(x)}} \exp\left[\int_a^b \kappa(x)\, dx\right] \exp\left[-\int_a^x \kappa(x')\, dx'\right] \tag{1.45}$$

and defining

$$\gamma \equiv \int_a^b \kappa(x)\, dx = \int_a^b \frac{\sqrt{2m\left[V(x) - E\right]}}{\hbar}\, dx, \tag{1.46}$$

the eq.(1.45) becomes

$$\psi_{II}(x) = \frac{-i}{\sqrt{\kappa(x)}} e^\gamma \exp\left[-\int_a^x \kappa(x')\, dx'\right]. \tag{1.47}$$

In region I, the solution of the Schrödinger equation is always an oscillating function. To make the calculation easier, and indicating as usual $k_0 \equiv \sqrt{2m(E - V_0)}/\hbar$, we shall write

$$\psi_I(x) = A\sin\left[k_0(x - a) + \varphi\right] = \frac{A}{2i}\left[e^{i[k_0(x-a)+\varphi]} - e^{-i[k_0(x-a)+\varphi]}\right]. \tag{1.48}$$

where the constants A and φ are determined by imposing the continuity of the wave function and of its derivative in $x = a$: in particular we find that

$$
\begin{cases}
k_0 \cot \varphi = -\kappa\left(a\right) \\
A \sin \varphi = \dfrac{-i}{\sqrt{\kappa\left(a\right)}} e^{\gamma}.
\end{cases}
\tag{1.49}
$$

As we want to study the tunnel effect through the potential barrier , we will be interested in the transmission coefficient T, given by the ratio between the transmitted probability current J_{III}^{tr} which reaches region III and the incident current J_I^{inc} coming from region I. In order to calculate J_I^{inc} let us note that ψ_I is the sum of an incident and reflected wave. It is easy to prove that [7]

$$
J \equiv \mathrm{Re}\left[\psi^*\left(x\right) \frac{\hat{p}}{m}\psi\left(x\right)\right] = \mathrm{Re}\left[\psi^*\left(x\right) \frac{\hbar}{im}\frac{d}{dx}\psi\left(x\right)\right].
$$

$$
J_I^{inc} = \frac{1}{4}\left|A\right|^2 \frac{\hbar k_0}{m} \quad \text{and} \quad J_{III}^{tr} = \frac{\hbar}{m}.
\tag{1.50}
$$

Using eq. (1.49) and (1.50), and performing few easy calculations, we get

$$
T = \frac{J_{III}^{tr}}{J_I^{inc}} = 4\frac{\sqrt{\left(V_a - E\right)\left(E - V_0\right)}}{V_a - V_0} e^{-2\gamma},
\tag{1.51}
$$

which means

$$
T \propto \exp\left[-\frac{2}{\hbar}\int_a^b \sqrt{2m\left[V\left(x\right) - E\right]}dx\right].
\tag{1.52}
$$

The reader may ask why we have used the WKB approximation. The reason is that we could not solve exactly the Schrödinger equation associated with the potential drawn in the previous figure. At the same time there was no small perturbative parameter associated with the potential which would allow us to use perturbative methods. Moreover we had potentials which (especially the Coulomb potential outside) were changing slowly on the scale of the wavelength involved, so it was the ideal ground to implement the WKB method.

---

[7] Let us remember that in one dimension the probability current is

$$
J \equiv \mathrm{Re}\left[\psi^*\left(x\right) \frac{\hat{p}}{m}\psi\left(x\right)\right] = \mathrm{Re}\left[\psi^*\left(x\right) \frac{\hbar}{im}\frac{d}{dx}\psi\left(x\right)\right].
$$