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# General solution of the Schrödinger equation. I

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**Abstract**

The wave equation in quantum mechanics and its general solution in the phase space are obtained.

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## INTRODUCTION

The Schrödinger wave (SW) equation in Quantum Mechanics (QM) is usually solved in terms of special functions or numerically. The general approach to solving the SW equation is to reduce its to the equation for hypergeometric function or some special function. To do that one needs to find first a special transformations for the wave function (w.f.) and its arguments to reduce the original equation to the hypergeometric form. However, the solution of the SW equation can be obtained in elementary functions.

We use here the abbreviation SW which means "Schrödinger's wave" function known as $\psi$-function. However, definition of a particle wave (wave of matter) was introduced by Louis De Broglie in 1924 known as particle-wave duality [1]. Definition of the De Broglie wavelength follows from some assumptions (chain of relations) for the photon:

$$E = h\nu, \quad c = \lambda\nu, \quad E = \frac{hc}{\lambda} = pc.$$

From this we obtain the definition of the $\lambda_B$ through the Planck constant $h$ and the relativistic momentum $p$ of the photon:

$$\lambda_B = \frac{h}{p}. \tag{1}$$

This definition is generalized for massive particles [2]. The momenta of relativistic particles depend on the mass and velocity $v$ by the formula:

$$p = mv\gamma \equiv \frac{mv}{\sqrt{1-(v/c)^2}}. \tag{2}$$

In non-relativistic approximation we have $p \simeq mv$.

The squared amplitude of the SW function ($\psi$-function) at a given point in the coordinate representation determines the probability density of finding the particle at this point. But the $\psi$-function is somewhat of a mystery. On the other hand, the De Broglie wave and the particle-wave duality are interpreted as a purely relativistic effect associated with *standing wave* moving with the particle [3]. The wave $\lambda_B$ is copmlitely deterministic and can be treated as the *classical wave* because it is expressed via the classical momentum $p$ and the constant $h$. The wave equation we derive and solve in this work is not the SW equation, but coinsides with the one. We develop a technics of direct quantization of the classical action.

## I. QUANTIZATION OF THE DE BROGLIE WAVE

Consider a simple mnemonic quantization using the De Broglie wave. We assume, as mentioned above and noted by many authors, that the De Broglie wave $\lambda_B$ is the standing

wave. If so, then this wave may have resonant frequences corresponding to the wavelengths equal to: $\lambda_R = \frac{1}{2}\lambda_B$, $\lambda_R = \lambda_B$, $\lambda_R = \frac{3}{2}\lambda_B \ldots$ The generalized expression can be written as

$$\lambda_R = \left(n + \frac{1}{2}\right)\lambda_B \equiv \left(n + \frac{1}{2}\right) h/p \tag{3}$$

or

$$p\bar{\lambda}_R = \left(n + \frac{1}{2}\right)\hbar, \quad n = 0,\, 1,\, 2, \ldots, \tag{4}$$

where $\bar{\lambda}_R = \lambda_R/2\pi$. This equation is similar to the quasiclassical quantization condition for two-turning-point problems [4].

Let us compare (4) with the Heisenberg's uncertainty principle,

$$\Delta x \Delta p \geq \hbar/2. \tag{5}$$

The minimal value of (4) is $p_0\bar{\lambda}_R = \hbar/2$ at $n = 0$ and is in agreemant with (5) if we put $\Delta x = \bar{\lambda}_{R_0}$, $\Delta p = p_0$; this is also true for $n > 0$ when $p > p_0$. Thus, (4) can be considered as a "decoding" of the Heisenberg's uncertainty principle if we put $\bar{\lambda}_R = \Delta x$, $p => \Delta p$. The standing waves can be described by the periodic functions $\cos(k_n x + \delta_n)$ or $\sin(k_n x + \delta_n)$, where $k_n$ are eigenvalues and $\delta_n$ are the corresponding phases.

## II. ONE-DIMENSIONAL SCHRÖDINGER EQUATION. FREE MOTION

The Schrödinger waves are described by the SW equation. Separable multi-dimensional problems are reduced to one-dimensional (1D) SW equations. The static 1D SW equation for a free particle of mass $m$ [4–6],

$$\frac{1}{2m}\left(-i\hbar\frac{d}{dx}\right)^2 \psi(x) = E\psi(x), \tag{6}$$

has a general solution in the form of a superposition of two plane waves in configuration space,

$$\psi(x) = C_1 e^{ikx} + C_2 e^{-ikx}. \tag{7}$$

Here $C_1$ and $C_2$ are (in general) complex constants, $k = p/\hbar$ is the wave number defined as $k = 2\pi/\lambda_B$ for the De Broglie wavelength $\lambda_B = h/p$ with the particle constant momentum $p = \sqrt{2mE}$, $h = 2\pi\hbar$ is the Plank's constant.

There is another approach to solving the SW equation. It is known that the SW equation can be derived with the help of the Bohr's correspondence principle [5]. This fundamental principle has been used at the stage of creation of quantum theory. It is used to establish correspondence between classical functions and operators of QM, and to derive the apparent

form of the operators. Moreover, the correspondence principle points out the way to a simplest solution of the SW equation.

The correspondence principle states that the laws of quantum physics must be so chosen that in the classical limit, where many quanta are involved, the quantum laws lead to the classical equations as an average. In this way, in [7] this principle has been used to derive the non-relativistic quasi-classical (QC) wave equation appropriate in the QC region and the relativistic QC wave equation [8].

We transform (6), which is the energy eigenvalue problem, to the equivalent form

$$\left(\frac{\hbar}{i}\frac{d}{dx}\right)^2 \psi(x) = p_E^2 \psi(x), \tag{8}$$

which is the problem on eigenvalues of $p_E^2 = (\hbar k)^2 = 2mE$, and introduce the dimensionless phase variable $\phi = p_E/\hbar = k_E x$. This gives the SW equation in the phase space,

$$\psi''_{\phi\phi} + \psi = 0, \tag{9}$$

which is the linear homogeneous second-order differential ($\mathrm{LHD}_2$) equation in canonical form. The general solution of this equation is given by a superposition of two plane waves in the phase space $\{\phi\}$,

$$\psi(\phi) = C_1 e^{i\phi} + C_2 e^{-i\phi}. \tag{10}$$

The dimensionless phase variable $\phi = kx = W/\hbar$ here is written in terms of the Hamilton's characteristic function $W = px$ (the reduced classical action) [9]. The purpose of this work is to show that the general solution of the SW equation for the case of an interacting particle has the same form (10) for the corresponding *reduced classical action* $W$.

## III. 1D SCHRÖDINGER EQUATION WITH INTERACTION

Quantum theory uses the concept of "action in QM". In the semiclassical approximation, the "action in QM" is used in the form of an expansion in terms of the Plank's constant $\hbar$: $S = S_0 + \hbar S_1 + \hbar^2 S_2 + \ldots$ [10]. But, in the quantization condition the *classical* action $S_0$ is used, and the corrections $S_1$, $S_2, \ldots$ have no physical meaning, but lead to artificial problems such as divergence of the solution at the turning points. In our approach the concept of "action in QM" is NOT necessary for the theory. Let us show that the SW equation and its solution can be obtained from the *classical* action [11].

In the general case of an interacting particle, we consider a conservative system when the Hamiltonian $H(x,\, p) = p^2/2m + V(x)$ is not an explicit function of time $t$ and equals to the total energy $E$, which is the constant of motion. In this case the Hamilton's principal

function is [9]

$$S(t,\,x) = -Et + W(x), \quad W(x) = \int^x p(x)dx, \tag{11}$$

where $W(x)$ is the Hamilton's characteristic function [9].

The SW equation in this case we write in the form

$$\left(\frac{\hbar}{i}\frac{d}{dx}\right)^2 \psi(x) = 2m[E - V(x)]\psi(x) \tag{12}$$

and seek solution of this equation resembling the plane wave as closely as possible:

$$\psi(t,\,x) = \psi_0 e^{iS(t,\,x)/\hbar}. \tag{13}$$

The first derivative of this function with respect to the variable $x$ is

$$\frac{d}{dx}\psi = \frac{i}{\hbar}\left(\frac{dW}{dx}\right)\psi \quad \Rightarrow \quad \frac{\hbar}{i}\frac{d}{dx}\psi = p(x)\psi, \tag{14}$$

where $(dW/dx) = p(x)$ is a generalalized momentum. The second derivative is

$$\frac{d^2}{dx^2}\psi = \left[\left(\frac{i}{\hbar}\right)^2 p^2(x) + \frac{i}{\hbar}\frac{dp}{dx}\right]\psi \quad \Rightarrow \quad \left(\frac{\hbar}{i}\frac{d}{dx}\right)^2 \psi(x) = \left[p^2(x) + \frac{\hbar}{i}\frac{dp}{dx}\right]\psi, \tag{15}$$

where $p^2(x) = 2m[E - V(x)]$.

The complex equality (15) gives the SW equation (12) if

$$\frac{\hbar}{i}\frac{dp}{dx} = 0 \quad \Rightarrow \quad \bar{p} = \text{const}, \tag{16}$$

What does this mean?

The operators in QM are Hermitian, i.e. their eigenvalues are real. The squared momentum operator $\hat{p}^2$ in the left hand side of (15) is Hermitian, if the condition (16) is met. The Plank's constant is *constant* value, not zero, hence, the derivative $p'_x = 0$. This means that the generalalized momentum $p(x)$ can only take discrete constant values, $\bar{p}$.

The condition (16) is the key one in solving the SW equation and supplies the *Hermiticity* of the squared momentum operator, $\hat{p}^2$, in (15). We emphasize that only if the condition (16) is satisfied, it is possible to obtain from (15) the SW equation (12).

Functions in mathematics can take both continuous and discrete values for specific values of argument. The condition (16) is a prerequisite for permitted movements in QM; it defines *allowed motions* or stationary states of a quantum system, i.e., the generalized momentum $p(x)$ can only take some constant discrete values (momentum eigenvalues $\bar{p}$).

Let me remind that to solve equations of motions in mechanics, it may be necessary to take into account some *constraints* that limit the motion of the system [9, p. 11]. For example, the beads of an abacus are constrained to 1D motion by the supporting wires.

Constraints may be classified in various ways. If constraints can be expressed as equations connecting the coordinates of particles (and possibly the time) having the form

$$f(\mathbf{r}_1, \mathbf{r}_2, \ldots, t) = 0,$$

then constraints are said to be *holonomic*. Constraints not expressible in this fashion are called *non-holonomic*. Typically, such constraints depend on the particle velocities (or momenta),

$$f(\mathbf{v}_1, \mathbf{v}_2, \ldots) = 0,$$

and possibly the coordinates.

This is a key point of our approach.

We treat the condition (16) as a *non-holonomic constraint*!

It restricts the movement of the particle so that the momentum is constant.

## IV. SOLUTION OF THE 1D SCHRÖDINGER EQUATION

Thus, equality (16) leads from (15) to the SW Eq. (12) and its general solution of the form:

$$\psi(\phi) = C_1 e^{i\phi} + C_2 e^{-i\phi}, \quad \phi(x) = \frac{1}{\hbar}\int^x p(x)dx. \tag{17}$$

The Schrödinger equation (12) can be written in the Sturm-Liouville canonical form [12],

$$\psi''_{xx} + [k^2 - U^2(x)]\psi = 0, \tag{18}$$

where

$k^2 = 2mE/\hbar^2$,

$U^2(x) = 2mV(x)/\hbar^2$,

$p^2(x) = \hbar^2[k^2 - U^2(x)] \equiv 2m[E - V(x)]$.

Transform (18) to the dimensionless phase variable $\phi(x) = W(x)/\hbar$. This can be done using the identity [13]

$$\frac{d}{dx}\left(f\frac{dy}{dx}\right) = \left(\sqrt{f}\frac{d^2}{dx^2} - \frac{d^2}{dx^2}\sqrt{f}\right)\left(\sqrt{f}y\right) \tag{19}$$

that gives the equation

$$\Psi''_{\phi\phi} + [1 - \delta(\phi)]\Psi = 0, \tag{20}$$

where $\Psi = \sqrt{p}\psi$. The function (functional)

$$\delta(\phi) = \frac{1}{\sqrt{p}}\frac{d^2\sqrt{p}}{d\phi^2} = \frac{1}{2}\frac{d\epsilon}{d\phi} + \frac{1}{4}\epsilon^2, \tag{21}$$

$$\epsilon = \frac{\hbar}{p^2}\frac{dp}{dx} \tag{22}$$

has the meaning of a potential in the phase space with the properties: 1) $\delta(\phi) = 0$ for $V(x) = 0$, 2) $\delta(\phi) \to \infty$ at the turning points (TPs) given by the Eq. $p(x) = 0$, 3) $\delta(\phi)$ is a small quantity of higher order at other points [10]. We can call (20) the SW equation in the phase space. The fulfillment of the inequality $\epsilon \ll 1$ is a necessary condition for the application of the QC approximation in QM.

The roots of the equation $p(x) = 0$ separate the classically allowed region where $p(x) \geq 0$ from the classically forbidden region where $p(x) < 0$. The function $\delta(\phi)$ in (20) has the properties of the $\delta$-function: according to (16) the quantity $\epsilon = k'_x/k^2 = p'_x/p^2 = 0$, therefore, $\delta(\phi) = 0$ excluding the TPs determined by the equality (16); in the TPs $\delta(\phi) \to \infty$. The corresponding equations in these regions follow from (20) and are given by the system in the phase space $\{\phi\}$ [14]

$$\begin{cases} \Psi''_{\phi\phi} + \Psi = 0, & p(x) > 0, \\ \Psi''_{\phi\phi} - \Psi = 0, & p(x) < 0. \end{cases} \tag{23}$$

The general solutions of these equations are

$$\begin{cases} \Psi(\phi) = Ae^{i\phi} + Be^{-i\phi}, & p(x) > 0, \\ \Psi(\phi) = Ce^{\phi} + De^{-\phi}, & p(x) < 0. \end{cases} \tag{24}$$

Solution in QM (w.f.) must be continuous and finite in the entire range $(-\infty, \infty)$. To build the physical solution in the entire range we need to merge the oscillating solution(s) in classically allowed region where $p(x) \geq 0$ with the exponentially decaying solution(s) in classically inaccessible regions where $p(x) < 0$ [7].

The functions (24) should smoothly merge into each other at the turning points. Matching these functions and their first derivatives at the turning point $x_k$ gives two equalities

$$\begin{cases} A + B = C + D, \\ iA - iB = -C + D, \end{cases} \tag{25}$$

which yield

$$\begin{cases} A = \left(Ce^{i\pi/4} + De^{-i\pi/4}\right)/\sqrt{2}, \\ B = \left(Ce^{-i\pi/4} + De^{i\pi/4}\right)/\sqrt{2}. \end{cases} \tag{26}$$

The connection formulas (26) supply the continuous transition of the general solutions (24) into each other at the turning point $x_k$.

The most popular and important in applications are the two-turning point (2TP) problems [7, 14]. For the 2TP problem, the entire interval $(-\infty, \infty)$ is divided by the TPs $x_1$ and $x_2$ into three regions. This leads with the help of the connection formulas (26) to the quantization condition [7, 14]

$$\int_{x_1}^{x_2} \sqrt{2m[E - V(x)]}dx = \pi\hbar\left(n + \frac{1}{2}\right). \tag{27}$$

The final solution for the 2TP problems (the state function) in the phase space is [14]

$$\Psi_n(\phi) = C_n \begin{cases} e^{\phi-\phi_1}, & x < x_1, \\ \sqrt{2}\cos(\phi - \phi_1 - \frac{\pi}{4}), & x_1 \le x \le x_2, \\ (-1)^n e^{-\phi+\phi_2}, & x > x_2, \end{cases} \tag{28}$$

where $\phi(n,\, x) = k_n x$, $\phi_1 = \phi(x_1) = -\pi(n+\frac{1}{2})/2$, $\phi_2 = \phi(x_2) = \pi(n+\frac{1}{2})/2$ [7]. Here we have took into account the fact that, for the stationary states, the phase-space variable $\phi(n,\, x)$ at the TPs $x_1$ and $x_2$ depends on quantum number $n$ and does not depend on the form of the potential. The normalization coefficient,

$$C_n = \sqrt{\frac{k_n}{\pi(n+\frac{1}{2})+1}}, \tag{29}$$

is calculated from the normalization condition $\int_{-\infty}^{\infty} |\psi_n(x)|^2\, dx = 1$.

The solution (28) describes *free motion* of a particle-wave in the enclosure (the enclosure being the interaction potential). Therefore, in bound state region, the interaction of the particle-wave with the potential reduces to reflection of the wave by "walls of the potential". The "classical" solution (28) is general for all types of 2TP problems and allows to solve multi-turning point problems which represent a class of the "insoluble" (by standard methods) problems with more than two turning points [8].

The oscillating part of (28),

$$\Psi_n(x) = \sqrt{\frac{2k_n}{\pi(n+\frac{1}{2})+1}}\cos\left(k_n x + \frac{\pi}{2}n\right), \tag{30}$$

has the form of a *standing wave*. The form of the phase variable $\phi(n,\, x) = k_n x + \pi n/2$ guaranties that the state functions $\Psi_n(\phi)$ are necessarily either symmetric $(n = 0, 2, 4, \ldots)$ or antisymmetric $(n = 1, 3, 5, \ldots)$. The function (30) corresponds to the principal term of the asymptotic series in theory of the $\mathrm{LHD}_2$ equations, which in QM gives the asymptote of the exact solution of the SW equation. The quantization condition (27) in our solution of the 1D SW equation (12) is not approximate. It is exact, i.e. (27) reproduces the exact energy spectra for *all* known solvable 2TP problems in QM [7, 14].

## V. THREE-DIMENSIONAL SCHRÖDINGER EQUATION

The case of three-dimensional (3D) problems was studied in our works [7, 13]. The derivation of the 3D wave equation (37) can be performed siminarly to 1D case given above. Consider the case of a central potential. In spherical coordinates, the variables are separated and the generating function is

$$\psi(t,\,\mathbf{r}) = Ce^{-i[Et-W(\mathbf{r})]/\hbar}, \tag{31}$$

where $W(\mathbf{r}) = W(r) + W(\theta) + W(\varphi)$. The first derivative gives

$$\vec{\nabla}\psi(t,\,\mathbf{r}) = \frac{i}{\hbar}(\vec{\nabla}W)\psi(t,\,\mathbf{r}). \tag{32}$$

The second derivative results in the SW equation,

$$\left[\frac{(-i\hbar\vec{\nabla})^2}{2m} + V(r)\right]\psi(\vec{r}) = E\psi(\vec{r}). \tag{33}$$

A QC analysis of (33) was performed [13]. The SW equation (33) was reduced to the form of the classical HJ equation. Separation of the resulting equation using the correspondence principle results in the three 1D equations in canonical form (18),

$$\left[\hbar^2\frac{d^2}{dr^2} + 2m(E-V) - \frac{\vec{M}^2}{r^2}\right]\mathrm{R}(r) = 0, \tag{34}$$

$$\left[\hbar^2\frac{d^2}{d\theta^2} + \vec{M}^2 - \frac{M_z^2}{\sin^2\theta}\right]\Theta(\theta) = 0, \tag{35}$$

$$\left[\hbar^2\frac{d^2}{d\varphi^2} + M_z^2\right]\Phi(\varphi) = 0, \tag{36}$$

where $\vec{M}^2 = (l+\frac{1}{2})^2\hbar^2$, $M_z^2 = m^2\hbar^2$ are the constants of separation and, at the same time, integrals of motion [7]. These equations are equivalent to the 3D equation

$$\left[(-i\hbar)^2\Delta^c + U(r)\right]\Psi(\vec{r}) = p_E^2\Psi(\vec{r}), \tag{37}$$

$$\Delta^c = \frac{\partial^2}{\partial r^2} + \frac{1}{r^2}\frac{\partial^2}{\partial\theta^2} + \frac{1}{r^2\sin^2\theta}\frac{\partial^2}{\partial\varphi^2}. \tag{38}$$

Here (37) is the wave equation in canonical form for the eigenvalue of the square of the momentum $p_E^2 = 2mE$; $\Delta^c$ is the canonical operator, $U(r) = 2mV(r)$. Note that (37) is not the SW equation, bun it can be called as the SW equation in canonical form. Solution of (37) reproduces the exact energy spectra for *all* known solvable 2TP problems in QM [7, 14, 15].

## CONCLUSION

1. We have shown that the Schrödinger wave equation can be derived using the classical action — the Hamilton's principal function; it is the key object in our approach. In our approach, there is no place for the concept "action in Quantum Mechanics".

2. We have obtained the Schrödinger equation in the phase space.

3. We have derived the connection formulas in the phase space using which we obtained the exact quantization condition for two-turning-point problems.

4. The general solution of the obtained equation is given by the superposition of two plane waves in the phase space.

5. We have generalized our approach for three-dimensional Schrödinger equation.

The same simple rules and the general solution formulated for two-turning-point problems can be applyed for multi-turning-point problems, as well. This approach can be easily generalized for the non-separable problems. Our approach can be considered as a general method for solving the Schrödinger equation.

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[1] L. de Broglie, Ann. Phys. **3**, 22 (1925)

[2] S. G. Fedosin, Hadr. Jour. **35**, 349 (2012)

[3] M. Sato and H. Sato, Phys. Essays **27**, 146 (2012)

[4] L. D. Landau and E. M. Lifshitz, *Quantum Mechanics (Non-Relativistic Theory)*, 3rd ed., Vol. 3 (Pergamon, 1977) iSBN: 978-0-08-020940-1

[5] D. Bohm, *Quantum Theory* (Dover Publications, New York, 1979)

[6] L. Schiff, *Quantum mechanics*, second ed. ed. (McGraw-Hill, New York, 1955)

[7] M. N. Sergeenko, Phys. Rev. **A53**, 3798 (1996), [arXiv: quant-ph/9911075]

[8] M. N. Sergeenko, Mod. Phys. Lett. **A12**, 2859 (1997), [arXiv:quant-ph/9911081]

[9] H. Goldstein, *Classical mechanics*, 2nd ed. (Addison-Wesly Publ. Comp., Reading, Massachusetts-Menlo Park-California-London- Amsterdam-Don Mills-Ontario-Sydney, 1999)

[10] N. Fröman and P. O. Fröman, *JWKB Approximation: Contributions to the Theory* (North Holland, Amsterdam, 1965)

[11] M. N. Sergeenko, "Zeroth wkb approximation in quantum mechanics," [arXiv:quant-ph/0206179v1] (2002), preprint UIC, UICHEP-TH/00-1, Chicago, 2000

[12] *Sturm-Lioville theory* (EMS Press, 2001)

[13] M. N. Sergeenko, Mod. Phys. Lett. A **15**, 83 (2000), [arXiv:quant-ph/9912069]

[14] M. N. Sergeenko, Int. J. Mod. Phys. A **18**, 1 (2003), [arXiv:quant-ph/0010084v2]

[15] M. N. Sergeenko, Eur. Phys. J. **C72**, 2128 (2012), [arXiv:hep-ph/1206.7099]