The Schrödinger equation from the point of view of the theory of stability.

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In 1926, Schrödinger published an article *"Quantization as an Eigenvalue Problem"* in which he proposed the equation that described the wave function ψ for a hydrogen atom

$$\frac{\hbar^2}{2m}\Delta\psi + (\varepsilon + \frac{e^2}{r})\psi = 0$$

In modern quantum mechanics, the Schrödinger equation is known as a postulate. However, Erwin Schrödinger, himself derived this equation applying the methods of classical mechanics. Schrödinger started his derivation with the Hamilton-Jacobi equation

$$H\left(q;\ \frac{\partial S}{\partial q}\right) = \varepsilon$$

Velocity and Hamilton's principal function S are related as follows

$$\vec{V} = (1/m_e)\nabla S$$

The usage of the Hamilton –Jacobi equation by Schrödinger was not accidental. He viewed a particle as a wave packet and search for a wave equation. The Hamilton-Jacobi method allows to reduce a classical problem of a particle’s motion to a partial differential equation.

For the motion of an electron in a hydrogen atom the H-J. Eq. has the following form

$$\frac{1}{2m}\left[\left(\frac{\partial S}{\partial x}\right)^2+\left(\frac{\partial S}{\partial y}\right)^2+\left(\frac{\partial S}{\partial z}\right)^2\right]-\frac{e^2}{r}=\varepsilon \qquad (1)$$

Schrödinger next introduced a function $\psi(\bar{r})=\exp\left(\frac{S}{\hbar}\right)$

He substituted $\psi(\bar{r})$ in the above form into Eq. (1) and obtained the following quadratic form

$$\left(\frac{\partial \psi}{\partial x}\right)^2+\left(\frac{\partial \psi}{\partial y}\right)^2+\left(\frac{\partial \psi}{\partial z}\right)^2-\frac{2m}{\hbar^2}\left(\varepsilon+\frac{e^2}{r}\right)\psi^2=0$$

Schrödinger next searched for a such function ψ that would give extreme value to the integral of the quadratic form

$$\delta\int dx\,dy\,dz\left[\left(\frac{\partial\psi}{\partial x}\right)^2+\left(\frac{\partial\psi}{\partial y}\right)^2+\left(\frac{\partial\psi}{\partial z}\right)^2-\frac{2m}{\hbar^2}\left(\varepsilon+\frac{e^2}{r}\right)\psi^2\right]=0$$

with an additional normalization condition $\int|\psi|^2\,d\tau=1$

The Euler–Lagrange equation for this variational problem turned out to be the Schrödinger equation

$$\frac{\hbar^2}{2m}\Delta\psi+(\varepsilon+\frac{e^2}{r})\psi=0$$

Errors in Schrödinger's derivation

This derivation was not accepted by the scientific community mainly for the following reasons

1) Schrödinger assumed $\psi(\bar{r})$ to be real, while the Schrödinger equation has complex solutions
2) When the substitution used by Schrödinger in his derivation was substituted back into the equation obtained by his mathematical procedure, it did not give the original Hamilton-Jacobi equation
3) Schrödinger used a variational principle, which physical meaning was not clear to the physicists.

However, S. Eq. gave a clear method for finding Bohr energy levels, and, therefore, it was taken as a postulate.

Schrödinger viewed an electron as a wave packet. He wrote: ‘It is, of course, strongly, suggested that we should try to connect ψ function with some *vibration process* in the atom’. Unfortunately, it was proven that an electron could not be modeled as a wave packet, because a wave packet spreads out, which contradicted the corpuscular behavior of a particle.

In the same year (1926) M. Born proposed the probabilistic interpretation of the wave function. Thus, mathematical ties with classical mechanics were broken.

The scientists who did not agree with the probabilistic interpretation of the wave function began to search for classical mechanics equations from which the Schrödinger equation would follow.

D.Bohm was a proponent of the causal interpretation to quantum mechanics. Bohm corrected the Schrödinger‘s first mistake. He represented ψ in the form

$$\psi = A \exp\left(iS/\hbar\right)$$

He substituted it into the S. Eq., separated real and imaginary parts, and obtained two equations

$$2(\nabla A)(\nabla S) + A\Delta S = 0 \qquad \frac{(\nabla S)^2}{2m} + U - \frac{\hbar^2}{2m}\frac{\Delta A}{A} = 0$$

We can see that the second Eq. looks like H-J Eq. but it contains besides the classical potential an additional term

Bohm called this term

$$-\frac{\hbar^2}{2m}\frac{\Delta A}{A} = U_Q$$ the “quantum potential”

Bohm’s erroneous interpretations.

(1) Bohm made an erroneous conclusion that

as $\hbar \longrightarrow 0$ $U_Q \to 0$

(2) Bohm assumed, that “*quantum potential effects do not necessary fall off with the distance…The quantum potential has the new feature of nonlocality implying an instantaneous connection between distant particles*”.

This Bohm’s assumption however is not supported by mathematical derivations

(3). The Bohm made wrong assumption: he believed that function U_Q has the same form on the entire space. However, the quantum potential has a concrete form only for those trajectories that satisfy the Schrödinger equation, and is different for different trajectories. Outside these trajectories, the form of the quantum potential is unknown.

$$U_Q = -\frac{\hbar^2}{2m}\frac{\Delta A}{A}$$

Let us go back to the derivation of the equation presented by Schrodinger and discuss the physical meaning of the variational principle he used.

As early as 1929 N.G. Chetaev, the well known expert in the theory of stability, assumed that the variational principle used by Schrödinger extracts from all the solutions of the H-J. Eq. only those solutions which are **stable.**

Chetaev studied the stability of the motion of a particle, under the same initial conditions but under the action of small perturbing forces. He introduced W, the potential energy associated with the perturbing forces, into H.J Eq.

$$\frac{(\nabla S)^2}{2m} + U + W = \varepsilon \qquad (1)$$

He assumed that the influence of the perturbing forces at an arbitrary point is proportional to the density of trajectories at that point. For stable trajectories this influence must be minimal

$$\iiint W A^2 d\tau = \iiint W \psi \psi^* d\tau \Rightarrow \min$$

This condition is equivalent to:

$$\delta \iiint \left(\frac{(\nabla S)^2}{2m} + U - \varepsilon \right) \psi \psi^* d\tau = 0 \qquad (2) \qquad\qquad \psi = A \exp\left(iS / \hbar \right)$$

This variational problem reduces to equation (3)

$$\iiint \left[\frac{\hbar^2}{2m}\left(\Delta\psi - \frac{\Delta A}{A}\psi \right) - (U-\varepsilon)\psi \right] d\tau\, \delta\psi^* = 0 \quad (3)$$

$$\frac{\hbar^2}{2m}\Delta\psi + (\varepsilon - U - \frac{\hbar^2}{2m}\frac{\Delta A}{A})\,\psi = 0 \quad (4)$$

Equation (4) looks like S. Eq, but it has additional term

$$-\frac{\hbar^2}{2\mathrm{m}}\frac{\Delta \mathrm{A}}{\mathrm{A}} = U_Q$$

That is Chetaev did not obtain the exact S. Eq. Also Chetaev like Bohm, erroneously believed that U_Q is the potential energy of small forces.

It is clear, that if we introduce an unknown potential Φ in H-J. Eq., such that Φ equals U_Q on stable trajectories, we obtain the exact Schrödinger Eq. I introduce Φ formally into the equation, without defining the physical meaning of potential Φ

H-J. Eq with additional term Φ has the form

$$\frac{(\nabla S)^2}{2m} + U + \Phi = \varepsilon$$

Now, using Chetaev's method, we consider the motion of a particle (or the center of mass of an extended object) under action of small perturbing forces with energy W. In this case the motion integral of a particle takes the form:

$$\frac{(\nabla S)^2}{2m} + U + \Phi + W = \varepsilon$$

The influence of the perturbing forces at an arbitrary point is proportional to the density of trajectories at that point. From point of view of the theory of stability, for stable trajectories this influence must be minimal.

$$\int W\psi\psi^{*}d\tau \Rightarrow \min, (5) \qquad \delta\iiint\left(\frac{(\nabla S)^{2}}{2m}+U+\Phi-\varepsilon\right)\psi\psi^{*}d\tau=0$$

This variational problem reduces to the follow equation

$$\iiint\left[\frac{\hbar^{2}}{2m}\left(\Delta\psi-\frac{\Delta A}{A}\psi\right)-(U+\Phi_{0}+A\frac{\partial\Phi}{\partial A}-\varepsilon)\psi\right]d\tau\,\delta\psi^{*}=0$$

If we take $\Phi_{o}=-\frac{\hbar^{2}}{2m}\frac{\Delta A}{A}=U_{Q}$ and $\partial\Phi/\partial A=0$ (*)

we obtain the S.Eq,

$$\frac{\hbar^{2}}{2m}\Delta\psi(\vec{r})+(\varepsilon-U)\psi(\vec{r})=0$$

In case of the hydrogen atom condition (*) extracts Bohr's orbits out of all solutions.

Hydrogen atom

Let us apply the above approach to a hydrogen atom.

The Schrödinger equation for the hydrogen atom

$$\nabla^2\psi + \frac{2m_e}{\hbar^2}\left(\varepsilon + \frac{e^2}{r}\right)\psi = 0 \qquad (1) \qquad \psi = A\exp(iS/\hbar) \qquad (2)$$

the solutions of S. equation are

$$\psi_{nlk}(r,\vartheta,\varphi) = A_{nlk}(r,\vartheta)\exp(ik\varphi)$$

The phase of the wave function is $S/\hbar = k\varphi$

Thus, for the velocity of the electron on the trajectories obtained from the Schrödinger equation we have

$$\bar{V} = \frac{1}{m_e}\nabla S = \frac{\hbar k}{m_e r\sin\vartheta}\bar{i}_\varphi$$

All trajectories are circular!

$$\nabla S = \frac{\partial S}{\partial r}\bar{i}_r + \frac{1}{r}\frac{\partial S}{\partial\vartheta}\bar{i}_\vartheta + \frac{1}{r\sin\vartheta}\frac{\partial S}{\partial\varphi}\bar{i}_\varphi$$

This result was confirmed with observation performed at the Institute AMOLF in the Netherlands.
The atom was placed in an electric field *E* and was excited by laser pulses.
They obtained with a photoionization microscope the picture of the **electron orbitals in a hydrogen atom**.
We can see that they all circular.

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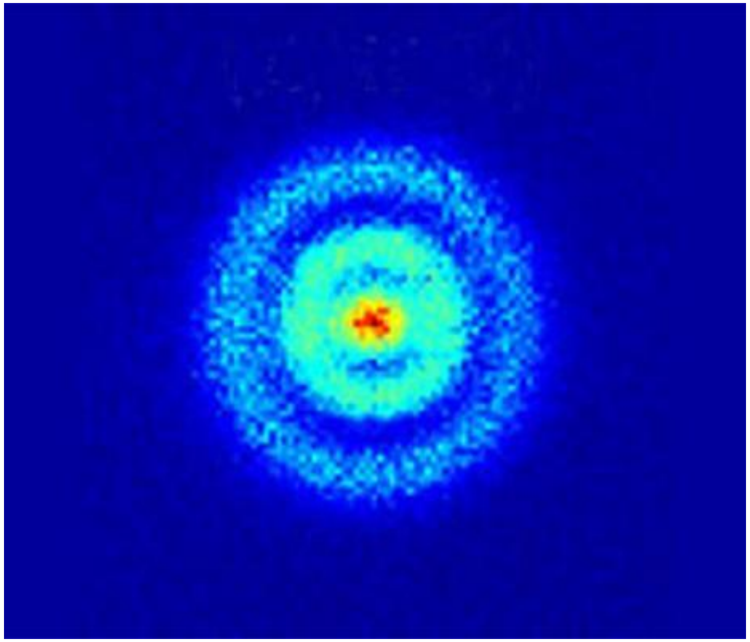

Note, that the motion on these circular trajectories satisfies only the necessary condition of stability, therefore, among these trajectories there are trajectories that are not stable. As I said before there is an additional condition for the stable trajectories

$\partial\Phi / \partial A = 0$ which has the form $\partial U_Q / \partial r = 0$

for the hydrogen atom.

It is this condition that extracts **Bohr orbits** as stable from all circular trajectories. This result follows directly from the theory of stability

$$r_{B_k} = \hbar^2 k^2 / m e^2 \qquad (7)$$

Conclusion

The H-J. Eq , $\frac{(\nabla S)^2}{2m} + U + \Phi = \varepsilon$ for the Bohr orbits takes form

$$\frac{m_e V_k^2}{2} - \frac{e^2}{r_{B_k}} + U_Q = \varepsilon_n \quad (8) \qquad \varepsilon_n = -\frac{e^4 m_e}{2\hbar^2 n^2}$$

For the center of mass we have

$$(1/2)\, m_e V_k^2 - e^2 / r_{B_k} = \varepsilon_k \quad (9)$$

If we compare formulas (8) and (9) we obtain

$$U_Q = \varepsilon_n - \varepsilon_k \qquad (10)$$

It can be seen that formula (10) is, in fact, **the Rydberg formula.**

The precession of the electron’s spin in an atom

$$\frac{m_e V_k^{\ 2}}{2} - \frac{e^2}{r_{B_k}} + U_Q = \varepsilon_n \quad (8)$$

Condition (8) is Jacobi’s integral of motion that contains not only energy of the center of mass

$$(1/2)\, m_e V_k^{\ 2} - e^2 / r_{B_k} = \varepsilon_k \quad (9)$$

but also the energy of rotational motion around the center of mass. In our case it is the precessional motion of the electron’s spin.

Thus, on the Bohr orbit “a quantum potential” equals to the energy of the precessional motion of the electron’s spin.