Field theoretic approach that forms a bijection between the wave mechanics and a space-time system obeying classical mechanics

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Abstract

At first, the classical particle motion of a general form will be interpreted in terms of the Hamiltonian densities, the kinetic energy density, the potential energy density and the sum of those, the total energy density. Secondly, the conditions for such Hamiltonian densities, which certainly will give rise to a classical particle motion, are then derived. The uniqueness of this density representation of Newton mechanics of a particle in terms of the equation of the Hamilton density becomes confirmed this way. The Hamiltonian densities given by the Schrödinger equation are studied next with this density representation of the classical mechanics as a tool. Those densities are found to be such Hamiltonian densities of a particle, which certainly will give rise to a classical particle motion obeying the classical mechanics. Thus a bijection between the wave mechanics and the classical particle system can be established. The classical particle trajectories obtained for such a Newtonian system are then discussed. The following working hypothesis is being used. Due to the bijection, the particle trajectories must be stochastic variables. Consequently, the location of the particle on a given trajectory must be a stochastic quantity. The reason is that the probability distribution given by the wave function must be unaltered. The probability to find a particle at a certain location on the trajectories is given by the wave function. Beneath of the information given by the wave mechanics, the properties of the particle on these trajectories are physical observables at certain observed points of the trajectories, because those properties are observables in an equivalent mechanical system. The constants of motion of the particle on the trajectory are exactly the quantum numbers of the corresponding eigenstate. Therefore the amount of information available from the quantum mechanical system is increased. The concept of the wave-particle duality and the concept of the complementarity principle become explained quantitatively and precisely in a natural way as a consequence of this bijection. The bijection to the classical particle system is obtained for both the time independent Schrödinger equation and the time dependent Schrödinger equation. The particle trajectories for a spherically symmetric Schrödinger equation are obtained. The particle trajectories for the hydrogen atom (hydrogen like atom) in the ground state and in the 2p-states are solved and can be compared with Compton scattering experiments. The nucleus O^{17} is considered as the next example. The trajectories for the valence neutron are

computed using Woods-Saxon shell model wave function giving rise to explicit expression for the kinetic energy of the neutron as a function of the nuclear radius. This data can be compared with experiments in the direct knock out reaction of the valence neutron in the reaction $O^{17}(p,np)O^{16}$ for instance. Thus, the nuclear shell model potential could then be extracted from such an experiment as a result. As an application of the time dependent theory, the particle trajectories for the one-dimensional linear harmonic oscillator in the time dependent polarized state of the ground state and the first exited state are obtained.

I. Introduction

Attempts have been made in order to improve the wave mechanics. This work is not an attempt to improve the quantum mechanics. It is an attempt to gain a better understanding of the wave mechanics, possibly enhance the amount of information to be observed from a quantum mechanical system and hopefully sharpen the picture to be obtained from a quantum mechanical system.

In Sec. II the classical particle motion of a general form is interpreted in terms of the energy density fields, the Hamiltonian density given as a sum of the kinetic energy density and potential energy density. The inambiquity of this interpretation is studied further in Sec. III. The question, what kind of Hamiltonian densities can interpret a classical particle motion, is studied there. The conditions for such a Hamiltonian density, given as a sum of the kinetic energy density and the potential energy density, which certainly gives rise to a classical particle motion, are described in Sec. III. Because the general classical particle motion is thus being formulated without any ambiguity in terms of the Hamiltonian densities, it is possible to compare the classical particle motion with those systems, where this kind of a representation is the usual procedure.

One well known system that is often interpreted in terms of the kinetic energy density, potential energy density and total energy density, is the Schrödinger equation. In Sec. IV the results of Sec. II and Sec. III are used. The equation of the Hamiltonian density obtained from the Schrödinger equation turns out to satisfy the conditions found in Sec. III. Hence, a classical particle motion can be determined for this system. Thus a bijection can be established between the Schrödinger equation and a certain space-time system obeying Newton mechanics. Because of this bijection, homomorphism exists between these systems. In Sec. V the classical particle trajectories of this space-time system are discussed briefly as consequences of this homomorphism.

The spherically symmetric time independent Schrödinger equation will be discussed in Sec. VI, such as the hydrogen atom for instance. Section VII is devoted to the time dependent Schrödinger

equation and to the equivalent classical system in this situation. Sections VIII, IX, and X discuss the hydrogen atom in its ground state, and in the 2p-states. In Sec. XI the polarized time dependent state of the linear harmonic oscillator is discussed as an application of the Sec. VII. The nucleus ^{17}O will be discussed in Sec. XII.

The classical harmonic oscillator is discussed in the Appendix as an application of the novel representation of the classical motion of the particle.

It will be mentioned already here, that a measurement of the particle coordinate for instance, would mean in this work a single observation of the particle position, a single click of the detector observing this quantity. The expectation value of this observable is the average of these observed values and this expectation value is often quoted with the phrase measurement. In this work a single click of the detector observing a given physical observable will be called a measurement of this observable.

II. Classical particle motion interpreted in terms of the energy density fields

Consider a conservative system, where the particle has the total energy E, the potential energy $U(\boldsymbol{x},t)$ and the kinetic energy $K(\boldsymbol{x},t)$ such, that

$$U(\boldsymbol{x},t) + K(\boldsymbol{x},t) = E \ . \tag{1}$$

We should find the expression of the potential energy density in terms of the potential energy $U(\boldsymbol{x},t)$. Evidently that would involve finding first the closed equipotential surfaces $S(\Omega)$, where the volume enclosed by the surface is denoted by Ω. Then the potential energy difference between two surfaces $S(\Omega)$ and $S(\Omega + d\Omega)$ of this kind and differing only infinitesimally from each other would be

$$dU = U(\Omega + d\Omega) - U(\Omega) . \tag{2}$$

On the other hand, the potential energy density $Vden(\Omega)$, which is a constant on the surface can be defined as

$$dU = Vden(\Omega) \cdot d\Omega \ . \tag{3}$$

The potential energy density obtained this way will be called subsequently the relative potential energy density $Vden(\Omega)$. This relative potential energy density can be obtained as the derivative

$$Vden(\Omega) = \frac{dU}{d\Omega} . \tag{4}$$

Defining the kinetic energy density in this way as well, will result the relative kinetic energy density as

$$Tden(\Omega) = -Vden(\Omega) . \tag{5}$$

This equation is obviously true everywhere and the two important equations are obtained

$$Tden(\boldsymbol{x},t) + Vden(\boldsymbol{x},t) = 0 \ , \tag{6}$$

$$Tden(\boldsymbol{x},t) = -Vden(\boldsymbol{x},t) \ . \tag{7}$$

These equations do not have any reference to some actual motion involving a given total energy and initial conditions of the particle motion. The kinetic energy $K(\boldsymbol{x},t)$ had its dependence on E as

$$K(\boldsymbol{x},t) = E - U(\boldsymbol{x},t) \ . \tag{8}$$

That dependence disappeared by differentiation. Consider again the equation for the relative fields

$$Tden(\boldsymbol{x},t) + Vden(\boldsymbol{x},t) = 0 \ \ . \tag{9}$$

Dividing the total energy E by the total volume Ωtot of the system will define the total energy density $\mathrm{H}_E(\boldsymbol{x},t)$ by

$$\mathrm{H}_E(\boldsymbol{x},t) = \frac{E}{\Omega tot} \ \ . \tag{10}$$

The contribution of the kinetic energy to the total energy in a classical system is the expectation value (the time average) of the kinetic energy. Denote the expectation value of the kinetic energy of a classical particle by $\langle\langle K \rangle\rangle$ and so, the average kinetic energy density of the system is

$$\mathrm{H}_K(\boldsymbol{x},t) = \frac{\langle\langle K \rangle\rangle}{\Omega tot} \ \ . \tag{11}$$

The average potential energy density is the time average of the potential energy U

$$\mathrm{H}_U(\boldsymbol{x},t) = \frac{\langle\langle U \rangle\rangle}{\Omega tot} \ \ . \tag{12}$$

The total average energy density $\mathrm{H}_E(\boldsymbol{x},t)$ becomes then defined as

$$\mathrm{H}_E(\boldsymbol{x},t) = \mathrm{H}_K(\boldsymbol{x},t) + \mathrm{H}_U(\boldsymbol{x},t) \ . \tag{13}$$

The addition of these numbers into the equation covering the relative densities (6) gives rise to the equation of the Hamiltonian density

$$\left[Tden(\boldsymbol{x},t) + \mathrm{H}_K(\boldsymbol{x},t)\right] + \left[Vden(\boldsymbol{x},t) + \mathrm{H}_U(\boldsymbol{x},t)\right] = \mathrm{H}_E(\boldsymbol{x},t) \ . \tag{14}$$

The bracketed expressions define the kinetic energy density $T(\boldsymbol{x},t)$ and the potential energy density $V(\boldsymbol{x},t)$ in the following way

$$T(\boldsymbol{x},t) = Tden(\boldsymbol{x},t) + \mathrm{H}_K(\boldsymbol{x},t), \tag{15}$$

$$V(\boldsymbol{x},t) = Vden(\boldsymbol{x},t) + \mathrm{H}_U(\boldsymbol{x},t) \ . \tag{16}$$

The equation of the Hamiltonian density takes the form

$$T(\boldsymbol{x},t) + V(\boldsymbol{x}t) = \mathrm{H}_E(\boldsymbol{x},t) \ . \tag{17}$$

This equation includes the information of the actual classical motion such, that the total energy is E and in addition, it is also telling that the expectation values of the kinetic energy and the potential energy are $\langle\langle K \rangle\rangle$ and $\langle\langle U \rangle\rangle$, respectively.

$$\langle\langle K\rangle\rangle = \int_0^{\Omega tot} \mathrm{H}_K(\boldsymbol{X},t)\cdot d\Omega \quad, \tag{18}$$

$$\langle\langle U\rangle\rangle = \int_0^{\Omega tot} \mathrm{H}_U(\boldsymbol{X},t)\cdot d\Omega \ , \tag{19}$$

and

$$E = \langle\langle K\rangle\rangle + \langle\langle U\rangle\rangle \ . \tag{20}$$

The relative energy densities measure the deviation of the actual density from the average. It is also obvious that there are infinitely many Hamiltonian densities of this type that can produce the same actual motion of the particle. Suppose the average kinetic energy density becomes defined as

$$\mathrm{H}_K(\boldsymbol{X},t) = \frac{\langle\langle K\rangle\rangle}{\Omega tot} + \Delta\mathrm{H}_K(\boldsymbol{X},t) \quad \text{such, that} \quad \int_0^{\Omega tot} \Delta\mathrm{H}_K(\boldsymbol{X},t)\cdot d\Omega = 0 \ . \tag{21}$$

The average potential energy density in turn is written as

$$\mathrm{H}_U(\boldsymbol{X},t) = \frac{\langle\langle U\rangle\rangle}{\Omega tot} + \Delta\mathrm{H}_U(\boldsymbol{X},t) \quad \text{such, that} \quad \int_0^{\Omega tot} \Delta\mathrm{H}_U(\boldsymbol{X},t)\cdot d\Omega = 0 . \tag{22}$$

When the kinetic energy and potential energy densities become defined as

$$\mathrm{T}(\boldsymbol{X},t) = Tden(\boldsymbol{X},t) + \mathrm{H}_K(\boldsymbol{X},t), \tag{23}$$

$$\mathrm{V}(\boldsymbol{X},t) = Vden(\boldsymbol{X},t) + \mathrm{H}_U(\boldsymbol{X},t), \tag{24}$$

and

$$\mathrm{H}_E(\boldsymbol{X},t) = \mathrm{H}_K(\boldsymbol{X},t) + \mathrm{H}_U(\boldsymbol{X},t) \ , \tag{25}$$

the equation for the Hamiltonian density will take the form

$$\left[Tden(\boldsymbol{X},t) + \mathrm{H}_K(\boldsymbol{X},t)\right] + \left[Vden(\boldsymbol{X},t) + \mathrm{H}_U(\boldsymbol{X},t)\right] = \mathrm{H}_K(\boldsymbol{X},t) + \mathrm{H}_U(\boldsymbol{X},t) \ . \tag{26}$$

The relative potential energy density $Vden(\boldsymbol{X},t)$ is obtained by subtracting the average potential energy density from the potential energy density. The relative kinetic energy density $Tden(\boldsymbol{X},t)$ is obtained by subtracting the average kinetic energy density from the kinetic energy density. Obviously the same relative densities are found as earlier. The same motion as earlier is obtained.

The densities $\Delta\mathrm{H}_K(\boldsymbol{X},t)$ and $\Delta\mathrm{H}_U(\boldsymbol{X},t)$ might represent the environment, the external system, turbulences, the medium, where the mechanical system is embedded in. This environment is such,

that the mechanical system remains unaltered, whenever $\Delta \mathrm{H}_K(\boldsymbol{x},t)$ and $\Delta \mathrm{H}_U(\boldsymbol{x},t)$ fulfils the conditions given in Eqs. (21) and (22) , respectively.

The question, how to find the motion of the particle, if the information of the particle motion is given entirely in the form of the Hamiltonian density

$$\mathrm{T}(\boldsymbol{x},t) + \mathrm{V}(\boldsymbol{x},t) = \mathrm{H}_E(\boldsymbol{x},t) , \tag{27}$$

will be discussed in the next Sec. III. Answer to the question will evidently involve the steps of this Sec. II but in reverse order.

III. The classical particle motion obtained from the equation of the Hamiltonian density

A. The description of the system

Consider a conservative system, where the particle has the kinetic energy density $T(\boldsymbol{x},t)$, the potential energy density $V(\boldsymbol{x},t)$ and the total average energy density $H_E(\boldsymbol{x},t)$ such that the equation of the Hamiltonian density is

$$T(\boldsymbol{x},t) + V(\boldsymbol{x},t) = H_E(\boldsymbol{x},t) \ . \tag{28}$$

The total average energy density $H_E(\boldsymbol{x},t)$ must be separable into two parts. The part $H_U(\boldsymbol{x},t)$ is arising entirely from the potential energy and $H_K(\boldsymbol{x},t)$ is arising from the kinetic energy of the system and

$$H_E(\boldsymbol{x},t) = H_K(\boldsymbol{x},t) + H_U(\boldsymbol{x},t). \tag{29}$$

The total energy of the system is a constant and given by the volume integral of $H_E(\boldsymbol{x},t)$ over all the space

$$E = \int_0^{\Omega_{tot}} H_E(\boldsymbol{x},t) \cdot d\Omega \ . \tag{30}$$

The expectation values of the kinetic energy and the potential energy of this particle motion are independent of the time and given by the integrals

$$\langle\langle K \rangle\rangle = \int_0^{\Omega_{tot}} H_K(\boldsymbol{x},t) \cdot d\Omega \ \ , \tag{31}$$

$$\langle\langle U \rangle\rangle = \int_0^{\Omega_{tot}} H_U(\boldsymbol{x},t) \cdot d\Omega \ \ , \tag{32}$$

$$E = \langle\langle K \rangle\rangle + \langle\langle U \rangle\rangle \ \ . \tag{33}$$

B. The solution of the classical particle motion

Restricting the consideration to the systems of this kind, a classical particle motion will be always obtained as will be shown next. The relative energy densities measured as deviations from the averages can be found as

$$\left[T(\boldsymbol{X},t) - H_K(\boldsymbol{X},t)\right] + \left[V(\boldsymbol{X},t) - H_U(\boldsymbol{X},t)\right] = 0, \tag{34}$$

where the bracketed expressions

$$Tden(\boldsymbol{X},t) = T(\boldsymbol{X},t) - H_K(\boldsymbol{X},t), \tag{35}$$

and

$$Vden(\boldsymbol{X},t) = V(\boldsymbol{X},t) - H_K(\boldsymbol{X},t), \tag{36}$$

will be called the relative kinetic energy density *Tden* and the relative potential energy density *Vden,* respectively.

These relative densities satisfy the equations

$$Tden(\boldsymbol{X},t) + Vden(\boldsymbol{X},t) = 0 \quad, \tag{37}$$

$$Tden(\boldsymbol{X},t) = -Vden(\boldsymbol{X},t) \quad. \tag{38}$$

The next thing to do, is to form the indefinite integral of the equation covering the relative energy densities, while the differential element of the integration is a differential volume element $d\Omega$. The primitives of the integrals are defined to be zero at boundary of the system. This differential volume element $d\Omega$ will be defined by the equidensity surfaces of the potential energy density *Vden*. Obviously these are also the equidensity surfaces of *Tden* as well.

Consider a closed surface $S(\Omega)$ such that the function *Vden* is a constant on this surface, the volume enclosed by the surface being denoted by Ω. Consider then another surface infinitesimally close to the earlier surface such, that the function *Vden* is a constant on this surface as well. Consider the volume of this surface and denote the volume enclosed by this surface by $\Omega + d\Omega$. Then the potential energy difference between the two surfaces is

$$dU = Vden(\boldsymbol{X},t) \cdot d\Omega \quad, \tag{39}$$

where $(\boldsymbol{X},t)$ is a point on the surface $S(\Omega)$. Thus, the indefinite integral $\int_{S(\Omega)} Vden(\boldsymbol{X},t) \cdot d\Omega + C2(t)$

is the value of the potential energy function on the surface $S(\Omega)$. This surface is one of those

surfaces, where the potential energy is a constant. The constant of integration *C2(t)* may depend only on time and is to be determined through the conditions of the motion. Forming the indefinite integral of the equation

$$Tden(\boldsymbol{x},t) + Vden(\boldsymbol{x},t) = 0 \tag{40}$$

will result

$$\left[\int_{S(\Omega)} Tden(\boldsymbol{x},t) \cdot d\Omega + C1(t) \right] + \left[\int_{S(\Omega)} Vden(\boldsymbol{x},t) \cdot d\Omega + C2(t) \right] = C3(t). \tag{41}$$

Interpreting the bracketed expressions as the kinetic energy and the potential energy, due to Eq. (39), the constant *C3(t)* is the total energy of the system, and the total energy is a constant in time.

$$\left[\int_{S(\Omega)} Tden(\boldsymbol{x},t) \cdot d\Omega + C1(t) \right] + \left[\int_{S(\Omega)} Vden(\boldsymbol{x},t) \cdot d\Omega + C2(t) \right] = E. \tag{42}$$

Because the primitives of the integrals are assumed to vanish at the boundary of the system,

$$C1(t) + C2(t) = E. \tag{43}$$

Given the potential energy at all equipotential surfaces $S(\Omega)$ defines the potential energy function in fact everywhere:

$$U(\boldsymbol{x},t) = \left[\int_{S(\Omega)} Vden(\boldsymbol{x'},t) \cdot d\Omega + C2(t) \right], \tag{44}$$

where $(\boldsymbol{x},t)$ is a point on the surface $S(\Omega)$. Similarly, the kinetic energy is found to be

$$K(\boldsymbol{x},t) = \left[- \int_{S(\Omega)} Vden(\boldsymbol{x'},t) \cdot d\Omega + C1(t) \right], \tag{45}$$

where $(\boldsymbol{x},t)$ is a point on the surface $S(\Omega)$.

Given the potential energy function, the equation of the motion can be written as

$$m \cdot \frac{d^2\boldsymbol{x}(t)}{dt^2} = -\nabla U(\boldsymbol{x}(t),t) \tag{46}$$

Consider the initial conditions for instance at boundary of the system and according to the equation

$$C1(0) + C2(0) = E. \tag{47}$$

There are two distinguishable cases to be discussed next.

If the physical system is such, that the particle would initially enter into the system in the asymptotic region at the boundary of the system and then, later on, would scatter out from the system in the asymptotic region at boundary of the system, the kinetic energies for the incoming and out coming particle must be the same in the conservative system. This asymptotic kinetic energy is obviously the expectation value of the kinetic energy $\langle\langle K \rangle\rangle$ and we must have $C1(0)=\langle\langle K \rangle\rangle$, and $C2(0)=\langle\langle U \rangle\rangle$. The trajectory of the particle is an open orbit.

If the physical system is such that the particle is moving on a closed orbit, the particle would have turning points at the boundary and the condition for the kinetic energy must be chosen accordingly.

The equation of motion for $\boldsymbol{x} = \boldsymbol{x}(t)$ can be solved in both cases and so, the expression for the kinetic energy $E_K(t)$) can be found as a function of time,

$$E_K(t) = \frac{1}{2} \cdot m \cdot \left(\frac{d}{dt}\boldsymbol{x}(t)\right)^2 .$$ (48)

On the other hand, the kinetic energy was given by Eq. (45),

$$E_K(t) = K(\boldsymbol{x}(t),t).$$ (49)

Using Eqs. (48) and (49) the constant of integration $C1(t)$ can be fully determined. Substituting the particle trajectory to the computed integral, the value of $C1(t)$ is obtained immediately as

$$C1(t) = E_K(t) + \left[\int_{S(\Omega)} Vden(\boldsymbol{x'},t) \cdot d\Omega\right]_{\boldsymbol{x} = \boldsymbol{x}(t)} .$$ (50)

The value of $C2(t)$ is consequently

$$C2(t) = E - E_K(t) - \left[\int_{S(\Omega)} Vden(\boldsymbol{x'},t) \cdot d\Omega\right]_{\boldsymbol{x} = \boldsymbol{x}(t)} .$$ (51)

Finally, the potential energy U and the kinetic energy K can be written as follows,

$$U(\boldsymbol{x},t) = \int_{S(\Omega)} Vden(\boldsymbol{x'},t) \cdot d\Omega + C2(t) ,$$ (52)

and

$$K(\boldsymbol{x},t) = - \int\limits_{S(\Omega)} Vden(\boldsymbol{x'},t) \cdot d\Omega + C1(t) \; , \tag{53}$$

where $(\boldsymbol{x},t)$ is any point on the arbitrary surface $S(\Omega)$. The constants of integration, *C1(t)* and *C2(t)*, are given by Eqs. (50 and 51), respectively.

C. The conditions for the Hamiltonian density

The conditions of the equation for the Hamiltonian density are given by the Eqs. (30) -(33). Those could look arbitrary. However, as will be shown next, those conditions will simply guarantee, somewhat surprisingly, that the equation of the Hamiltonian density obtained this way will be exactly the one found in Sec. II for the classical particle motion of a general form. That equation became defined there in Sec. II with aid of the Eqs. (10) -(17).

The following definitions will be made first

$$H_K = \frac{\langle\langle K \rangle\rangle}{\Omega tot} + H_K - \frac{\langle\langle K \rangle\rangle}{\Omega tot} \; , \tag{54}$$

$$H_K = \frac{\langle\langle K \rangle\rangle}{\Omega tot} + \Delta H_K \; , \tag{55}$$

and

$$\Delta H_K = H_K - \frac{\langle\langle K \rangle\rangle}{\Omega tot} \; . \tag{56}$$

Defined in this way, the density ΔH_K is such, that the condition given by the Eq. (21) is satisfied, i.e.,

$$\int\limits_0^{\Omega tot} \Delta H_K \cdot d\Omega = 0 \; . \tag{57}$$

Writing the identity

$$T = T - H_K + \frac{\langle\langle K \rangle\rangle}{\Omega tot} + H_K - \frac{\langle\langle K \rangle\rangle}{\Omega tot} \; , \tag{58}$$

and observing, that by definition $Tden = T - H_K$, the expression of the kinetic energy density T is found to be

$$T = Tden + \frac{\langle\langle K \rangle\rangle}{\Omega tot} + \Delta H_K \; . \tag{59}$$

A similar consideration as the one above, will yield also the potential energy density V as

$$V = Vden + \frac{\langle\langle U \rangle\rangle}{\Omega tot} + \Delta H_U \quad . \tag{60}$$

In this Eq. (60) the average potential energy density is written as

$$H_U = \frac{\langle\langle U \rangle\rangle}{\Omega tot} + \Delta H_U \quad . \tag{61}$$

The density ΔH_U in the Eq.(61) is given by

$$\Delta H_U = H_U - \frac{\langle\langle U \rangle\rangle}{\Omega tot} \quad . \tag{62}$$

Also this density ΔH_U satisfies the condition given by the Eq. (22), i.e.,

$$\int_0^{\Omega tot} \Delta H_U \cdot d\Omega = 0 \quad . \tag{63}$$

The substitution of the expressions of T, V, H_U and H_K of Eqs. (59), (60), (61), and (55), respectively, into the equation of the Hamiltonian density given by the Eqs. (28) and (29) ,yields

$$\left[Tden + \frac{\langle\langle K \rangle\rangle}{\Omega tot} + \Delta H_K \right] + \left[Vden + \frac{\langle\langle U \rangle\rangle}{\Omega tot} + \Delta H_U \right] = \left[\frac{\langle\langle K \rangle\rangle}{\Omega tot} + \Delta H_K \right] + \left[\frac{\langle\langle U \rangle\rangle}{\Omega tot} + \Delta H_U \right] . \tag{64}$$

Cancelling ΔH_K and ΔH_U from this equation, the remaining equation for the Hamiltonian density is given by

$$\left[Tden + \frac{\langle\langle K \rangle\rangle}{\Omega tot} \right] + \left[Vden + \frac{\langle\langle U \rangle\rangle}{\Omega tot} \right] = \left[\frac{\langle\langle K \rangle\rangle}{\Omega tot} \right] + \left[\frac{\langle\langle U \rangle\rangle}{\Omega tot} \right] . \tag{65}$$

This is exactly the same equation for the Hamiltonian density, which was obtained for the classical particle motion of a general form in Sec. II, being interpreted there in Eqs. (10)-(17). The uniqueness of the representation of the classical particle motion in terms of the equation of the Hamiltonian density is confirmed.

IV. The time independent Schrödinger equation

The time independent Schrödinger equation will be written as

$$(\widehat{T} + \widehat{V}) \cdot \phi(\boldsymbol{x}) = E \cdot \phi(\boldsymbol{x}) \ . \tag{66}$$

The total energy in the eigenstate $\phi(\boldsymbol{x})$ is written as a sum of the expectation values of the potential energy and the kinetic energy

$$E = \langle \widehat{T} \rangle + \langle \widehat{V} \rangle \ . \tag{67}$$

The probability density is denoted by $\rho(\boldsymbol{x})$ and expressed as

$$\rho(\boldsymbol{x}) = \phi^*(\boldsymbol{x}) \cdot \phi(\boldsymbol{x}) \ . \tag{68}$$

Multiplying the Schrödinger equation from the left by $\phi^*(\boldsymbol{x})$ and substituting $E = \langle \widehat{T} \rangle + \langle \widehat{V} \rangle$ will result

$$\phi^*(\boldsymbol{x}) \cdot \widehat{T} \cdot \phi(\boldsymbol{x}) + \widehat{V} \cdot \rho(\boldsymbol{x}) = \langle \widehat{T} \rangle \cdot \rho(\boldsymbol{x}) + \langle \widehat{V} \rangle \cdot \rho(\boldsymbol{x}) \ . \tag{69}$$

The following definitions will be made below. The kinetic energy density $T(\boldsymbol{x})$, the potential energy density $V(\boldsymbol{x})$, the average total energy density $H_E(\boldsymbol{x})$, the average potential energy density $H_U(\boldsymbol{x}$, and the average kinetic energy density $H_K(\boldsymbol{x})$, respectively, are defined in the following way:

$$T(\boldsymbol{x}) = \phi^*(\boldsymbol{x}) \cdot \widehat{T} \cdot \phi(\boldsymbol{x}), \tag{70}$$

$$V(\boldsymbol{x}) = \widehat{V} \cdot \rho(\boldsymbol{x}) \ , \tag{71}$$

$$H_E(\boldsymbol{x}) = E \cdot \rho(\boldsymbol{x}) \ , \tag{72}$$

$$H_U(\boldsymbol{x}) = \langle \widehat{V} \rangle \cdot \rho(\boldsymbol{x}) \ , \tag{73}$$

$$H_K(\boldsymbol{x}) = \langle \widehat{T} \rangle \cdot \rho(\boldsymbol{x}) \ , \tag{74}$$

and

$$H_E(\boldsymbol{x}) = H_K(\boldsymbol{x}) + H_U(\boldsymbol{x}) \ . \tag{75}$$

The equation of the Hamiltonian density will follow using the Schrödinger equation, as follows,

$$T(\boldsymbol{x}) + V(\boldsymbol{x}) = H_E(\boldsymbol{x}) \ . \tag{76}$$

The equations (72), (73), (74), and (75) yield finally, using the eqs. (30), (31), (32), and (33),

$$\langle\langle K \rangle\rangle = \langle \widehat{T} \rangle, \tag{77}$$

$$\langle\langle U \rangle\rangle = \langle \widehat{V} \rangle, \tag{78}$$

and

$$E = \langle\langle K \rangle\rangle + \langle\langle U \rangle\rangle. \tag{79}$$

These conditions satisfy quite obviously the requirements of Sec. III, given by Eqs. (28)-(33), for an equation of the Hamiltonian density of a classical particle, obeying the laws of the Newton mechanics. The conditions written down there are fulfilled. Classical particle motion can be obtained as was done in Sec. III. The derivations of the earlier Sec. III are not repeated here.

To begin with, the relative densities are

$$Vden(\boldsymbol{x}) = \left(\widehat{V} - \langle\langle U \rangle\rangle \right) \cdot \rho(\boldsymbol{x}), \tag{80}$$

$$Tden(\boldsymbol{x}) = \phi^*(\boldsymbol{x}) \cdot \widehat{T} \cdot \phi(\boldsymbol{x}) - \langle\langle K \rangle\rangle \cdot \rho(\boldsymbol{x}). \tag{81}$$

The next step is to form the indefinite integral of both sides of the equation

$$Tden(\boldsymbol{x}) + Vden(\boldsymbol{x}) = 0 \tag{82}$$

such, that the differential element of the integration is $d\Omega$ (see Eq. (39) for the definition) and the primitives of the integrals are chosen to be zero on the boundary of the system,

$$\left[\int_{S(\Omega)} Tden(\boldsymbol{x}) \cdot d\Omega + C1 \right] + \left[\int_{S(\Omega)} Vden(\boldsymbol{x}) \cdot d\Omega + C2 \right] = C3. \tag{83}$$

The identification of the expressions inside the brackets as the kinetic energy and the potential energy will fix the constant on the right hand side to be $C3=E$. The constant of the integration on the left has been divided into two parts, $C1$ and $C2$, just for convenience. The exception of the general case considered in the earlier Sec. III is, that the relative energy densities are independent of time. For this reason the constants of integration are also taken to be independent of time.

Consider the case mentioned in Sec. III, when the particle was assumed to enter and to leave the boundary of the system at the asymptotic speed on an open orbit. The asymptotic kinetic energy is $\langle\langle K \rangle\rangle$ and hence the constants of integration are found immediately,

$$\left[\int_{S(\Omega)} Tden(\boldsymbol{x}) \cdot d\Omega + \langle\langle K \rangle\rangle \right] + \left[\int_{S(\Omega)} Vden(\boldsymbol{x}) \cdot d\Omega + \langle\langle U \rangle\rangle \right] = E \ . \tag{84}$$

The potential energy U and the kinetic energy K are obtained on the surface $S(\Omega)$. The values of the potential energy U and the kinetic energy K are constant on this surface. In the expressions below the radius vector $\boldsymbol{x}$ in U and K is an arbitrary vector such, that its end point is on the surface $S(\Omega)$,

$$U_{S(\Omega)}(\boldsymbol{x}) = \int_{S(\Omega)} \left[\hat{V} - \langle\langle U \rangle\rangle\right] \cdot \rho \cdot d\Omega + \langle\langle U \rangle\rangle \ , \tag{85}$$

and

$$K_{S(\Omega)}(\boldsymbol{x}) = - \int_{S(\Omega)} \left[\hat{V} - \langle\langle U \rangle\rangle\right] \cdot \rho \cdot d\Omega + \langle\langle K \rangle\rangle \ . \tag{86}$$

Extending the computation such, that the surfaces $S(\Omega)$ will fill the whole space, the potential energy and the kinetic energy functions are obtained everywhere in the space.

Using the boundary conditions, the asymptotic kinetic energy being $\langle\langle K \rangle\rangle$, the equation of the motion can be solved and the trajectories $\boldsymbol{x}(t)$ of the particle can be evaluated using the equation of the motion,

$$m \cdot \frac{d^2 \boldsymbol{x}(t)}{dt^2} = -\nabla U(\boldsymbol{x}(t)) \ . \tag{87}$$

On the other hand, it is obvious, that if this system of classical mechanics is fully known, the following functions, the kinetic energy K of Eq. (86) and the potential energy U of Eq. (85) are also known functions. The quantum mechanical system can be constructed using the method described in the earlier Sec. II. The approach described in Sec. II will yield the relative densities $Vden$ and $Tden$. Because $Vden$ is related with the density $\rho(\boldsymbol{x})$ by the Eq. (80),

$$Vden(\boldsymbol{x}) = \left(\hat{V} - \langle\langle U \rangle\rangle\right) \cdot \rho(\boldsymbol{x}) \ , \tag{88}$$

the probability density $\rho(\boldsymbol{x})$, and hence, the wave function can be determined.

Thus, the present description offers a bijection from the wave mechanics to a system in the space-time obeying the laws of the classical mechanics.

However, the phrases like the motion, the trajectory, the propagation on the trajectory, could be misleading. Some discussion about the physical significance of these concepts will be presented in the next section.

V. The particle trajectories

It will be mentioned repeatedly here, that a measurement of the particle coordinate for instance, would mean in this work a single observation of the particle position, a single click of the detector observing this quantity as was mentioned already in Sec. I. It does not mean the expectation value.

It is absolutely impossible to conclude exactly the physical significance of the particle trajectories without specific experimental guidance and so the discussion about the physical significance would remain on the level of speculation. The following working hypothesis will be used instead.

The particle does not propagate smoothly along these trajectories in the space-time, but the trajectory itself and the more so, a specific point on the trajectory is a stochastic variable. The reason is that the probability distribution is given by the wave function and the probability distribution must remain unaltered in all circumstances. The probability to find the particle on some point on the trajectory is given by the wave function. The current description is nothing but quantum mechanics; this is what the current working hypothesis is stating in brief. The probability distribution is not altered, the expectation values remain unaltered, and those are given by the wave mechanics. The constants of motion of the particle on the trajectory are exactly the same as the quantum numbers in the corresponding eigenstate.

Further, once found localized at a certain point on the trajectory, the position and the velocity of the particle are both measurable and predictable simultaneously according to the specific trajectory in question. This is true on some point on some trajectory of the present description; the number of possible trajectories in the system can be infinite. If the trajectories belonging to a given eigenstate fill the whole space-time we have the situation that could have been described in the wave mechanics by the concept of the wave particle duality. In addition to the information given by the wave mechanics the system has predictable particle-like properties observable all over the space-time. Examples of systems of this kind to be considered later in this work are the hydrogen atom in the 1s-state and the linear harmonic oscillator in a polarized time-dependent state.

On the other hand, in some other state, the particle trajectories might not extend all over in the space-time. The hydrogen atom in the 2p-state to be considered later is one example of this kind of a system. This is the situation that might have been described up to now in the wave mechanics by the concept of the complementarity principle. In other words, according to this work, beneath of the wave mechanical description, this kind of a system has predictable particlelike properties in some well defined regions of the space-time.

One could also speculate that the particle trajectories might also serve as gates into a certain state of the system. If a localized particle has coordinates and momenta corresponding to a certain point on the trajectory of a certain quantum mechanical state, the particle might get delocalized immediately into that state in question. This guess is not being included in the working hypothesis about the physical significance of the particle trajectories.

VI. The time independent spherically symmetric Schrödinger equation

Consider again the equation for the densities, Eq. (82),

$$Tden(\boldsymbol{x}) + Vden(\boldsymbol{x}) = 0 \ . \tag{89}$$

Substitute first

$$\phi = u(r) \cdot Y_{lm}(\theta, \varphi) \tag{90}$$

to obtain

$$\left[u(r) \cdot \left[-\frac{\hbar^2}{2 \cdot m} \frac{d^2}{dr^2} + \frac{\hbar^2 \cdot l \cdot (l+1)}{2 \cdot m \cdot r^2} - \langle \widehat{T} \rangle \right] u(r) + \left[V(r) - \langle \widehat{V} \rangle \right] \cdot u(r)^2 \right] \cdot \left(Y_{lm} \right)^* \cdot Y_{lm} = 0 \ . \tag{91}$$

Here $\langle \widehat{T} \rangle = \langle\langle K \rangle\rangle$ and $\langle \widehat{V} \rangle = \langle\langle U \rangle\rangle$ [see Eqs. (77) and (78)].

The equation (91) gets simplified by noticing, that the equation is true if $u(r)$ is the solution of the radial Schrödinger equation. Because $\left(Y_{lm} \right)^* \cdot Y_{lm}$ may in this case be anything, and $\left(Y_{lm} \right)^* \cdot Y_{lm}$ depends only on θ, the equation is true for all values of θ between 0 and π and so we have

$$\begin{cases} u(r) \cdot \left[-\frac{\hbar^2}{2 \cdot m} \frac{d^2}{dr^2} + \frac{\hbar^2 \cdot l \cdot (l+1)}{2 \cdot m \cdot r^2} - \langle \widehat{T} \rangle \right] u(r) + \left[V(r) - \langle \widehat{V} \rangle \right] \cdot u(r)^2 = 0 \\ \theta, \varphi = anything \end{cases} \tag{92}$$

From Eq. (92) follows, that it is enough to consider radial relative energy densities $Vden(r)$ and $Tden(r)$ only. Denote

$$Vden(r) = \left[V(r) - \langle \widehat{V} \rangle \right] \cdot u_{nl}(r)^2 \tag{93}$$

and

$$Tden(r) = -Vden(r) \tag{94}$$

The surfaces of constant density are the same for both $Tden$ and $Vden$. Below, $d\Omega$ is denoting the infinitesimal volume difference between two infinitesimally different equidensity surfaces of the relative radial potential energy density $Vden$. How to obtain this differential volume element will be discussed in detail later in the case of the hydrogen atom. The integration will yield the potential

energy U and the kinetic energy K on the spherical surfaces S(Ω). These surfaces S(Ω) are also surfaces, where the potential energy is a constant. The potential energy is found to be

$$U(r) = \int_{S(\Omega)} \left[V(r) - \langle\widehat{V}\rangle\right] \cdot \rho_{nl}(r) \cdot d\Omega + \langle\widehat{V}\rangle , \tag{95}$$

where

$$\rho_{nl}(r) = u_{nl}(r)^2 . \tag{96}$$

The kinetic energy is obtained simply with aid of the potential energy,

$$K(r) = - \int_{S(\Omega)} \left[V(r) - \langle\widehat{V}\rangle\right] \cdot \rho_{nl}(r) \cdot d\Omega + \langle\widehat{T}\rangle = E - U(r). \tag{97}$$

Because of the spherical symmetry, the Lagrangian of the system becomes

$$L = \frac{1}{2} \cdot m \cdot \left(\frac{dr}{dt}\right)^2 + \frac{1}{2} \cdot m \cdot r^2 \cdot \left(\frac{d\phi}{dt}\right)^2 - U(r) . \tag{98}$$

Because the Lagrangian has spherical symmetry, the classical particle orbit will be in a plane. For this reason ϕ is the polar angle in that plane and θ is a constant. The spherical polar coordinate r of the particle takes now the role of the polar radius in that plane. The value of θ will be chosen below. Because ϕ is a cyclic coordinate, the angular momentum, defined as the generalized momentum corresponding to ϕ , is a conserved quantity. Among the initial conditions there is the conservation of the angular momentum:

$$m \cdot r^2 \cdot \frac{d\phi}{dt} = constant = \pm\sqrt{\hbar^2 \cdot l \cdot (l+1)} \tag{99}$$

Let the unit vector $\boldsymbol{n}$ be the normal vector of the plane of the motion such, that

$$n_z = \sin(\theta), \tag{100}$$

$$m \cdot r^2 \cdot \frac{d\phi}{dt} \cdot \boldsymbol{n} = \boldsymbol{L} = \pm\sqrt{\hbar^2 \cdot l \cdot (l+1)} \cdot \boldsymbol{n} \quad \text{and so} \quad \left|\boldsymbol{L}\right|^2 = \hbar^2 \cdot l \cdot (l+1). \tag{101}$$

The value of $\theta = constant$, the spherical coordinate of the particle, will be fixed such, that

$$L_z = \left|\boldsymbol{L}\right| \cdot \sin(\theta) \cdot sign(\frac{d\phi}{dt}) = \hbar \cdot m . \tag{102}$$

The initial condition for the radial velocity may be obtained directly from the expression of the kinetic energy as

$$K(r) = \frac{1}{2} \cdot m \cdot \left(\frac{dr}{dt}\right)^2 + \frac{\hbar^2 \cdot l \cdot (l+1)}{2 \cdot m \cdot r^2} . \tag{103}$$

The trajectories of the particle are solvable simply by solving the following first order equations (and choosing the signs accordingly).

$$\frac{dr}{dt} = \sqrt{\frac{2 \cdot K(r)}{m} - \frac{\hbar^2 \cdot l \cdot (l+1)}{m^2 \cdot r^2}} \quad \text{or} \quad \frac{dr}{dt} = -\sqrt{\frac{2 \cdot K(r)}{m} - \frac{\hbar^2 \cdot l \cdot (l+1)}{m^2 \cdot r^2}} \quad , \tag{104}$$

$$\frac{d\phi}{dt} = \frac{\sqrt{\hbar^2 \cdot l \cdot (l+1)}}{m \cdot r^2} \quad \text{or} \quad \frac{d\phi}{dt} = -\frac{\sqrt{\hbar^2 \cdot l \cdot (l+1)}}{m \cdot r^2} \quad . \tag{105}$$

It is worth of noticing, that the constants of motion of the classical particle motion found in this section, are exactly the same as the quantum numbers in the quantum mechanical state.

VII. The time dependent Schrödinger equation

Consider the time dependent Schrödinger equation

$$(\widehat{T} + \widehat{V}) \cdot \psi = i \cdot \hbar \cdot \frac{\partial \psi}{\partial t} \ . \tag{106}$$

The energy densities will be obtained by multiplying from the left by ψ^* and forming then the complex conjugate of the equation obtained so far. The aim is to resolve the real and imaginary parts of the energy densities.

$$\psi^* \cdot (\widehat{T} + \widehat{V}) \cdot \psi = i \cdot \hbar \cdot \psi^* \cdot \frac{\partial \psi}{\partial t} \ , \tag{107}$$

$$\psi \cdot (\widehat{T} + \widehat{V}) \cdot \psi^* = -i \cdot \hbar \cdot \psi \cdot \frac{\partial \psi^*}{\partial t} . \tag{108}$$

Denote

$$\rho = \psi^* \cdot \psi \ . \tag{109}$$

The expression of the kinetic energy density is complex and the imaginary part is simply

$$\frac{i \cdot \hbar}{2} \cdot \nabla \cdot \boldsymbol{j} \ . \tag{110}$$

Here is the explicit expression of the kinetic energy density:

$$\psi^* \cdot \widehat{T} \cdot \psi = \frac{1}{2} \cdot (\psi^* \cdot \widehat{T} \cdot \psi + \psi \cdot \widehat{T} \cdot \psi^*) + \frac{i \cdot \hbar}{2} \cdot \nabla \cdot \boldsymbol{j} \ . \tag{111}$$

Similarly, the total energy density includes an imaginary part being

$$\frac{i \cdot \hbar}{2} \cdot \frac{\partial \rho}{\partial t} \tag{112}$$

The total energy density can be written as

$$\psi^* \cdot i \cdot \hbar \cdot \frac{\partial \psi}{\partial t} = \frac{i \cdot \hbar}{2} \cdot (\psi^* \cdot \frac{\partial \psi}{\partial t} - \psi \cdot \frac{\partial \psi^*}{\partial t}) + \frac{i \cdot \hbar}{2} \cdot \frac{\partial \rho}{\partial t} \ . \tag{113}$$

The equation considering the imaginary part of the energy densities is simply the continuity equation multiplied by $\frac{i \cdot \hbar}{2}$. It is automatically satisfied, when ψ is a solution of the time dependent

Schrödinger equation. Because the imaginary kinetic energy is not an observable, it is enough to consider the real part of the energy densities. If it would be necessary to construct, for some reason, the quantum mechanical state starting from the classical mechanics, then also this imaginary part could be used in order to help getting the complex phases of the wave function correctly.

The equation for the real parts of the energy densities is

$$\frac{1}{2} \cdot (\psi^* \cdot \widehat{T} \cdot \psi + \psi \cdot \widehat{T} \cdot \psi^*) + \widehat{V} \cdot \rho = \frac{i \cdot \hbar}{2} \cdot (\psi^* \cdot \frac{\partial \psi}{\partial t} - \psi \cdot \frac{\partial \psi^*}{\partial t}) \ . \tag{114}$$

Denote the total average energy on the right hand side of Eq. (114) density by $H_E(\boldsymbol{X},t)$. This density satisfies then the equation:

$$\frac{1}{2} \cdot (\psi^* \cdot \widehat{T} \cdot \psi + \psi \cdot \widehat{T} \cdot \psi^*) + \widehat{V} \cdot \rho = H_E(\boldsymbol{X},t) \ . \tag{115}$$

The expressions of the kinetic energy density and the potential energy density, respectively, can be found from the Eq. (115) as follows

$$T(\boldsymbol{X},t) = \frac{1}{2} \cdot (\psi^* \cdot \widehat{T} \cdot \psi + \psi \cdot \widehat{T} \cdot \psi^*) \ , \tag{116}$$

and

$$V(\boldsymbol{X},t) = \widehat{V} \cdot \rho(\boldsymbol{X},t) \ . \tag{117}$$

On the other hand, instead of Eq. (115), $H_E(\boldsymbol{X},t)$ can be written as the right hand side of Eq. (114):

$$H_E(\boldsymbol{X},t) = \frac{i \cdot \hbar}{2} \cdot (\psi^* \cdot \frac{\partial \psi}{\partial t} - \psi \cdot \frac{\partial \psi^*}{\partial t}) \ . \tag{118}$$

Next, the total average energy density $H_E(\boldsymbol{X},t)$ will be expressed as a sum,

$$H_E(\boldsymbol{X},t) = H_K(\boldsymbol{X},t) + H_U(\boldsymbol{X},t), \tag{119}$$

to be calculated using the expression

$$H_E(\boldsymbol{X},t) = \frac{i \cdot \hbar}{2} \cdot (\psi^* \cdot \frac{\partial \psi}{\partial t} - \psi \cdot \frac{\partial \psi^*}{\partial t}) \ . \tag{120}$$

Writing the wave function as a superposition of the eigenstates

$$\psi(\boldsymbol{X},t) = c_1 \cdot \phi_1(\boldsymbol{X}) \cdot e^{\frac{-i \cdot E_1 \cdot t}{\hbar}} + c_2 \cdot \phi_2(\boldsymbol{X}) \cdot e^{\frac{-i \cdot E_2 \cdot t}{\hbar}} , \tag{121}$$

the expression of $H_E(\boldsymbol{X},t)$ given above by Eq. (120) can be evaluated.

 Even though this expression (121) is a truncated form of the general expression of the wave function $\psi(\boldsymbol{X},t))$, this restriction will cause no loss of generality in the conclusions and in the algorithm that is being developed. Extension to the general superposition of the eigenstates will be transparent. This truncated form of the wave function must not be understood as an approximation.

The parts arising from the kinetic energy and from the potential energy will be separated in the expression of the total energy density $H_E(\boldsymbol{X},t)$ by denoting $\omega = (E_2 - E_1)/\hbar$ and defining:

$$H_E = E_1 \cdot |c_1|^2 \cdot |\phi_1|^2 + E_2 \cdot |c_2|^2 \cdot |\phi_2|^2 + (E_2 + E_1) \cdot \mathrm{Re}\left[c_1^* \cdot c_2 \cdot \phi_1^* \cdot \phi_2 \cdot e^{-i \cdot \omega \cdot t} \right] ,$$
(122)

$$H_K = T_1 \cdot |c_1|^2 \cdot |\phi_1|^2 + T_2 \cdot |c_2|^2 \cdot |\phi_2|^2 + (T_2 + T_1) \cdot \mathrm{Re}\left[c_1^* \cdot c_2 \cdot \phi_1^* \cdot \phi_2 \cdot e^{-i \cdot \omega \cdot t} \right] ,$$
(123)

and

$$H_U = V_1 \cdot |c_1|^2 \cdot |\phi_1|^2 + V_2 \cdot |c_2|^2 \cdot |\phi_2|^2 + (V_2 + V_1) \cdot \mathrm{Re}\left[c_1^* \cdot c_2 \cdot \phi_1^* \cdot \phi_2 \cdot e^{-i \cdot \omega \cdot t} \right] .$$
(124)

Above, the energy of the eigenstate ϕ_1 is being denoted by E_1, and has been expressed as a sum of the expectation values in that state as

$$E_1 = T_1 + V_1 \ .$$
(125)

Of course,

$$E_2 = T_2 + V_2 \quad .$$
(126)

Now we have the equation

$$T(\boldsymbol{X},t) + V(\boldsymbol{X},t) = H_E(\boldsymbol{X},t) \ ,$$
(127)

where $T(\boldsymbol{X},t)$ is the kinetic energy density, $V(\boldsymbol{X},t)$ is the potential energy density and $H_E(\boldsymbol{X},t)$ the average total energy density. The average total energy density can be written as

$$H_E(\boldsymbol{X},t) = H_K(\boldsymbol{X},t) + H_U(\boldsymbol{X},t).$$
(128)

The terms in the sum in Eq. (128), given by Eqs. (123) and (124), separate the contributions of the kinetic energy and the potential energy in the expression of the average total energy density given by Eq. (122). The quantum mechanical expectation value, like the one of the kinetic energy operator

$\widehat{T}$ for instance, $\langle \widehat{T} \rangle$ might include off-diagonal matrix elements of the eigenstates in a general case. Because the following identification must be done

$$\langle\langle K \rangle\rangle = |c_1|^2 \cdot T_1 + |c_2|^2 \cdot T_2 \ , \tag{129}$$

$$\langle\langle U \rangle\rangle = |c_1|^2 \cdot V_1 + |c_2|^2 \cdot V_2 \ , \tag{130}$$

and consequently $\langle \widehat{T} \rangle \neq \langle\langle K \rangle\rangle$, in general. However, here is precisely the system described in Sec. III. When the energy E of the classical system is identified to be $E = \langle \widehat{H} \rangle$, one obtains

$$\langle\langle K \rangle\rangle + \langle\langle U \rangle\rangle = \langle \widehat{H} \rangle = E \ . \tag{131}$$

The conditions for the Hamiltonian density, which are given by the Eqs. (28)-(33) in Sec. III, are all satisfied. A classical particle motion can be obtained in this system. The method, written down in Sec. III, will be used for this purpose.

First, the relative energy densities *Vden* and *Tden* must be determined,

$$Vden(\boldsymbol{x},t) = \widehat{V} \cdot \rho - \mathrm{H}_U(\boldsymbol{x},t), \tag{132}$$

$$Tden(\boldsymbol{x},t) = \frac{1}{2} \cdot (\psi^* \cdot \widehat{T} \cdot \psi + \psi \cdot \widehat{T} \cdot \psi^*) - \mathrm{H}_K(\boldsymbol{x},t). \tag{133}$$

The consideration may proceed exactly in the same way as in Sec. III. The next step is to form the indefinite integral of the both sides of the equation

$$Tden(\boldsymbol{x},t) + Vden(\boldsymbol{x},t) = 0 \ . \tag{134}$$

The differential element of the integration is $d\Omega$ [defined earlier by Eq. (39) in Sec. III]. The primitives of the integrals are chosen to be zero on the boundary of the system. The constants of the integration may depend on time.

$$\left[\int_{S(\Omega)} Tden(\boldsymbol{x},t) \cdot d\Omega + C1(t) \right] + \left[\int_{S(\Omega)} Vden(\boldsymbol{x},t) \cdot d\Omega + C2(t) \right] = C3(t) \ . \tag{135}$$

Interpreting the expressions inside the brackets as the kinetic energy and the potential energy of the system, the constant of the integration $C3(t)$ represents the total energy of the system. The total energy of this classical system is $\langle H \rangle = E$ as was discussed above in Eq. (131). Then,

$$C3(t) = \langle H \rangle = E, \tag{136}$$

and

$$\left[\int_{S(\Omega)} Tden(\boldsymbol{X},t) \cdot d\Omega + C1(t) \right] + \left[\int_{S(\Omega)} Vden(\boldsymbol{X},t) \cdot d\Omega + C2(t) \right] = E \ . \tag{137}$$

Because the primitives of the integrals are taken to vanish at the boundary of the system, one obtains

$$C1(t) + C2(t) = E \ , \tag{138}$$

$$U(\boldsymbol{X},t) = \int_{S(\Omega)} Vden(\boldsymbol{X'},t) \cdot d\Omega + C2(t) \ , \tag{139}$$

Such a computation as the one above, will yield the potential energy U, and the kinetic energy K, for that matter, at any point $(\boldsymbol{X},t)$ on the surface $S(\Omega)$. Hence, the potential energy is found in fact everywhere.

This is the case of Sec. III, when the particle would enter into the system across the boundary of the system at asymptotic speed and it would also leave the system across the boundary at asymptotic speed. That speed is given by the expectation value of the kinetic energy $\langle\langle K \rangle\rangle$ of the classical system defined above in Eq. (129). The equation of the motion reads:

$$m \cdot \frac{d^2\boldsymbol{X}(t)}{dt^2} = -\nabla U(\boldsymbol{X}(t),t) \tag{141}$$

together with the condition on the boundary of the system:

$$\frac{1}{2} \cdot m \cdot v_x{}^2 + \frac{1}{2} \cdot m \cdot v_y{}^2 + \frac{1}{2} \cdot m \cdot v_z{}^2 = \langle\langle K \rangle\rangle \ . \tag{142}$$

As can be seen, the constant of integration $C2(t)$ has no effect on the particle motion. Once the trajectory $\boldsymbol{X}(t)$ of the particle is obtained, the kinetic energy $E_K(t)$ of the particle as a function of time can be determined as

$$E_K(t) = \frac{1}{2} \cdot m \cdot \left(\frac{d\boldsymbol{x}(t)}{dt} \right)^2 \quad . \tag{143}$$

On the other hand, the kinetic energy is given by the Eq. (140) as

$$E_K(t) = K(\boldsymbol{x}(t),t), \tag{144}$$

and so, the constant of integration *C1(t)* can be determined. Substituting the particle trajectory into the computed integral of the equation (7.33), the value of *C1(t)* is obtained immediately as

$$C1(t) = E_K(t) + \left[\int_{S(\Omega)} Vden(\bar{x}',t) \cdot d\Omega \right]_{\boldsymbol{x} = \boldsymbol{x}(t)} . \tag{145}$$

The value of *C2(t)* is consequently

$$C2(t) = \langle H \rangle - E_k(t) - \left[\int_{S(\Omega)} Vden(\bar{x}',t) \cdot d\Omega \right]_{\boldsymbol{x} = \boldsymbol{x}(t)} . \tag{146}$$

When *C1(t)* and *C2(t)* are given by the Eqs. (145) and (146), respectively, the potential energy function and the kinetic energy function of the classical particle can be written as follows,

$$U(\boldsymbol{x},t) = \int_{S(\Omega)} Vden(\boldsymbol{x}',t) \cdot d\Omega + C2(t) , \tag{147}$$

$$K(\boldsymbol{x},t) = \int_{S(\Omega)} Tden(\boldsymbol{x}',t) \cdot d\Omega + C1(t) . \tag{148}$$

In these equations the point $(\boldsymbol{x},t)$ is any point on the arbitrary surface $S(\Omega)$. However, the constants of integration *C1(t)* and *C2(t)* were obtained using a certain trajectory, with given initial conditions.

On the other hand, if the classical system is known, the functions *U* and *K* given in the Eqs. (147) and (148) are fully known. The quantum mechanical state can be obtained as follows. The application of the approach of Sec. II would first yield the functions $Vden(\boldsymbol{x},t)$, and $Tden(\boldsymbol{x},t)$, which are independent of the constants of integration *C1(t)* and *C2(t)*. The following two equations are obtained with these known functions on the left hand side,

$$Vden(\boldsymbol{x},t) = \hat{V} \cdot \rho - H_U(\boldsymbol{x},t) , \tag{149}$$

$$Tden(\boldsymbol{x},t) = \frac{1}{2} \cdot (\psi^* \cdot \hat{T} \cdot \psi + \psi \cdot \hat{T} \cdot \psi^*) - H_K(\boldsymbol{x},t) \tag{150}$$

In addition, there is the continuity equation

$$\nabla \cdot \boldsymbol{j} = \frac{\partial \rho}{\partial t} \tag{151}$$

It is obvious, that the superposition of the wave function can be resolved using these three equations.

Thus the present description offers a bijection from the wave mechanics to the space-time system obeying classical mechanics also in the case of the time dependent Schrödinger equation.

As an application of this section, the linear harmonic oscillator in a polarized state of the ground state and the first exited state as a function of time will be considered later in Sec. XI.

VIII. The ground state of the hydrogen atom

The Coulomb potential is spherically symmetric and hence the computation of the trajectories of the electron in the hydrogen atom will proceed as was described in Sec. VI. The Coulomb potential is written as

$$V(r) = -\frac{k}{r} \; , \tag{152}$$

where

$$k = 1.43992 \cdot 10^{-9} \cdot eV \cdot m \; . \tag{153}$$

The energy levels of the hydrogen atom are given by

$$E_n = -\frac{1}{2 \cdot n^2} \cdot \frac{k}{a} \; , \tag{154}$$

where a is the Bohr radius

$$a = 0.529172 \cdot 10^{-10} \cdot m \; . \tag{155}$$

The radial wave function for the ground state of the hydrogen atom is

$$u(r)_{1,0} = \sqrt{\frac{4}{a^3}} \cdot r \cdot e^{-\frac{r}{a}} \; . \tag{156}$$

This wave function is subject to the normalization condition

$$\int_0^\infty \left[\sqrt{\frac{4}{a^3}} \cdot r \cdot e^{-\frac{r}{a}} \right]^2 \cdot dr = 1 \; . \tag{157}$$

The expectation value of the potential energy is

$$E_p = -\frac{k}{a} \; . \tag{158}$$

The relative potential energy density is (see Fig.1)

$$Vden(r) = \left(\sqrt{\frac{4}{a^3}} \cdot r \cdot e^{-\frac{r}{a}} \right)^2 \cdot \left(-\frac{k}{r} - \frac{-k}{2 \cdot a} \right) , \tag{159}$$

and the relative kinetic energy density is in turn

$$Tden(r) = -Vden(r) \ . \tag{160}$$
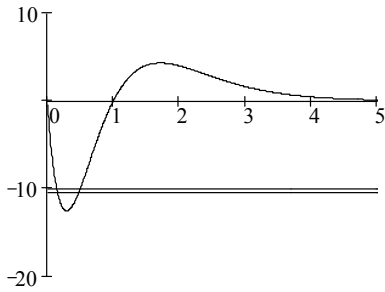
FIG. 1. The relative potential energy density times a as a function of $x=r/a$. Two equidensity surfaces are indicated with two horizontal lines. The horizontal axis is in eV.
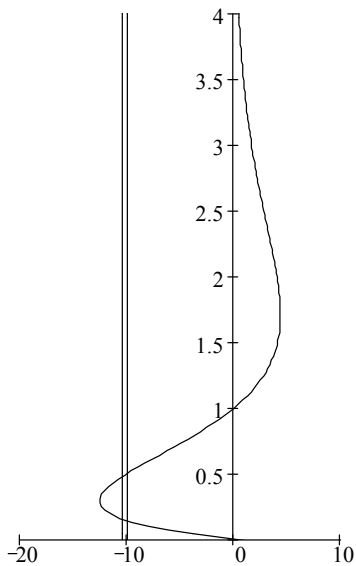
FIG. 2. The inverse function of the potential energy density as a function of the potential energy density times a. The horizontal axis is in units $x=r/a$ and the vertical axis is in eV.

In this essentially one-dimensional case the differential element $d\Omega$ in Eq. (95) is the difference in the lengths of the segments connecting points of equal density in Fig. 2. Denote by *rmin* and *rmax* the positions of the minimum and the maximum of the function *Vden(r)* and denote by *rzero* the position of the zero-point of this function. An algorithm will be developed next, which is suitable to compute the potential energy $U(r)$, and the kinetic energy $K(r)$.

Denote by $x = f(\varepsilon,0)$ the branch of the inverse function of *Vden* in Fig. 2, when *0<r<rmin*, and denote by $x = f(\varepsilon,1)$ the branch of the inverse function of *Vden* in Fig. 2, when *rmin<r<rmax* . Denote the values of the relative potential energy density *Vden(r)* at *rmin* and *rmax* by εmin and εmax , respectively.

Then $d\Omega$ is obtained here, for convenience, as a function of ε , the potential energy density as

$$d\Omega = (f'(\varepsilon,1) - f'(\varepsilon,0)) \cdot d\varepsilon \text{ , when } 0 < r < rzero \tag{161}$$

Then the potential energy as a function of ε in the interval *0<r<rzero* can be written as

$$V_\varepsilon(\varepsilon,1) = \int_0^\varepsilon \varepsilon \cdot \left[\frac{df(\varepsilon,1)}{d\varepsilon} - \frac{df(\varepsilon,0)}{d\varepsilon} \right] \cdot d\varepsilon + \langle V \rangle \text{ ,} \tag{162}$$

where $d\Omega$ was chosen to be negative. Integrating by parts yields

$$V_\varepsilon(\varepsilon,1) = \varepsilon \cdot (f(\varepsilon,1) - f(\varepsilon,0)) - \int_0^\varepsilon (f(\varepsilon,1) - f(\varepsilon,0)) \cdot d\varepsilon + \langle V \rangle \text{ .} \tag{163}$$

Because $\varepsilon = Vden(r)$ when *0<r<rzero*, the potential energy as a function of *r* in the interval *0<r<rzero* can be obtained by the following substitution:

$$U(r) = V_\varepsilon(Vden(r),1) + \langle V \rangle \text{ , when } 0 < r < rzero \text{ .} \tag{164}$$

Denoting by $x = f(\varepsilon,2)$ the branch of the inverse function in Fig. 2, when *rmax<r<∞* , the potential energy in that interval takes the form

$$V_\varepsilon(\varepsilon,2) = \varepsilon \cdot (f(\varepsilon,2) - f(\varepsilon,2)) - \int_0^\varepsilon (f(\varepsilon,2) - f(\varepsilon,2)) \cdot d\varepsilon + \langle V \rangle \text{ ,} \tag{165}$$

where $d\Omega$ was chosen to be negative again. The whole potential energy function as a function of *r* will be obtained by the following substitution:

$$U(r) = V_\varepsilon(Vden(r),2) + \langle V \rangle \text{ , when } rzero < r < \infty \text{ .} \tag{166}$$

The kinetic energy is then

$$K(r) = E - U(r) \text{ .} \tag{167}$$

The trajectories are now easy to obtain using Eq. (104). The particle trajectories simply pass radially through the atom and the angular momentum is zero. The total energy of the classical particle is exactly the total energy of the eigenstate. The results of the computation are shown in the graphs in Fig. 3, Fig. 4, and Fig. 5 below.
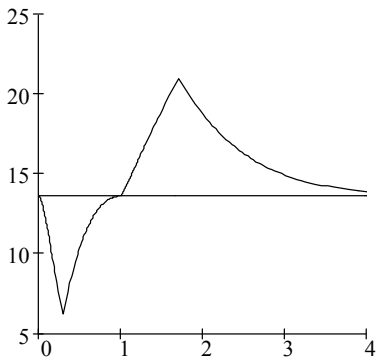

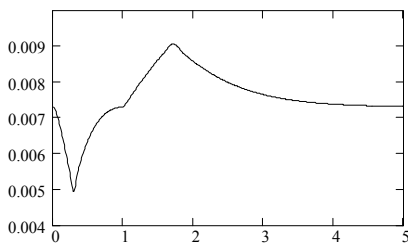FIG.3. The kinetic energy in the 1s-state in *eV* as a function of *r/a*. The horizontal dashed line is the expectation value of the kinetic energy.

FIG. 4. The positive radial velocity divided by the speed of light, the vertical axis, as a function of *r/a*, the horizontal axis.
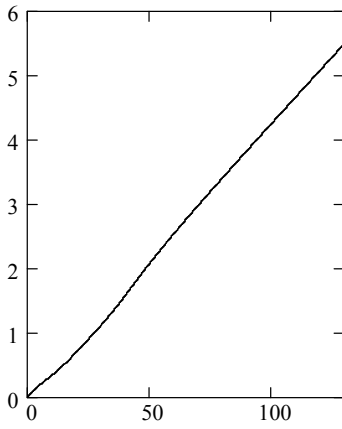
FIG. 5. The vertical axis: the radial distance of the particle from the origin in units of the Bohr radius on a trajectory, as a function of time. The horizontal axis: the time in attoseconds.

IX. The 2p, m=0 state of the hydrogen atom

In the 2p-state of the hydrogen atom, the relative radial potential energy density is

$$Vden(r) = \left[\sqrt{\frac{4}{3 \cdot a}} \cdot \left(\frac{r}{a} \right)^2 \cdot e^{-\frac{r}{a}} \right]^2 \cdot \left[\frac{-k}{r} - \frac{-k}{2 \cdot a} \right] \quad . \tag{168}$$

The total energy is

$$E = -\frac{-k}{8 \cdot a} \quad . \tag{169}$$

The expectation value of the kinetic energy is

$$E_K = \frac{3 \cdot k}{8 \cdot a} \quad , \tag{170}$$

and the expectation value of the potential energy is in turn

$$E_P = \frac{-k}{2 \cdot a} \quad . \tag{171}$$

The computation of the potential energy and the kinetic energy will proceed in a manner similar to the 1s-state. Both $U(r)$ and $K(r)$ can be found using the same algorithm as in the 1s –state. The kinetic energy is graphed below in Fig. 6. The kinetic energy of the radial motion can be seen in Fig. 7 below.
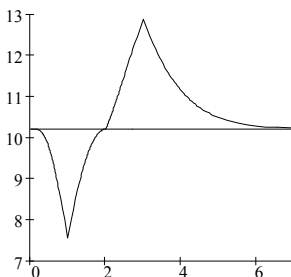
FIG. 6. The vertical axis: the kinetic energy of the electron in the 2p-state as a function of r/a. The energy is in eV. The horizontal line is the expectation value of the kinetic energy.
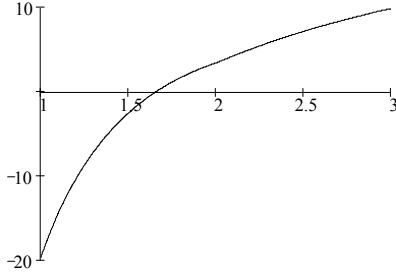
FIG. 7. The kinetic energy of the radial motion in eV is plotted as a function of r/a in the graph. The radial kinetic energy becomes zero at the distance r_1 from the origin. Due to the angular momentum conservation the particle trajectory cannot get closer to the origin than r_1. The radius r_1 is in the 2p-state about 1.7 times the Bohr radius.

Following the discussion of Sec. VI, the Lagrangian of the system is written as

$$L = \frac{1}{2} \cdot m \cdot \left(\frac{dr}{dt}\right)^2 + \frac{1}{2} \cdot m \cdot r^2 \cdot \left(\frac{d\phi}{dt}\right)^2 - U(r) \ , \tag{172}$$

and $\theta_0 = 0$ or $\theta_0 = \pi$ for particles in the upper or lower half space, respectively.

Because ϕ is a cyclic coordinate,

$$m \cdot r^2 \cdot \frac{d\phi}{dt} = \pm\hbar\sqrt{2} \ , \tag{173}$$

i.e., the angular momentum is a constant of the motion.

The initial conditions of the motion starting at (r_0, ϕ_0) at $t=0$ can be written as

$$\frac{1}{2} \cdot m \cdot vr_0^2 + \frac{1}{2} \cdot m \cdot r_0^2 \cdot \omega_0^2 = K(r_0) \ , \tag{174}$$

$$m \cdot r_0^2 \cdot \omega_0 = \pm\hbar \cdot \sqrt{2} \ . \tag{175}$$

The total angular momentum is set to be $\pm\hbar \cdot \sqrt{2}$, thus defining $\dfrac{d\phi}{dt}$ for the given total angular momentum. The initial radial velocity is vr_0 and the initial value of $\dfrac{d\phi}{dt}$ is ω_0. The angular momentum squared is $2 \cdot \hbar^2$. The path of the particle will be always in some plane through the origin such, that the plane is perpendicular to the xy-plane and hence $L_z = 0$. This is why $\theta_0 = 0$ or

$\theta_0 = \pi$ as was discussed Sec. VI. The particle could propagate on the trajectory either with positive

angular velocity $\dfrac{d\phi}{dt} > 0$ or with negative angular velocity $\dfrac{d\phi}{dt} < 0$, always $L_z = 0$. The geometric

shape and the time dependence of the trajectory is always the same in all 2p-states. A typical

trajectory can be seen in Fig. 8.

Here is an example of the complementarity principle of the quantum mechanics: Beneath of the
picture predicted by the wave mechanics, the particle has in this L=1, m=0 state mechanical
properties of a classical particle, when localized outside the sphere of the radius r_1. See Fig. 8
below. It has mechanical properties of a classical particle in the following sense. When localized at
certain point in the space-time, its velocity and position are given by the trajectory passing through
that point. The probability to find the particle on some of these trajectories is given just by the
probability density of the wave function and is *1-P(r_1)=0.759* . The probability to find the particle
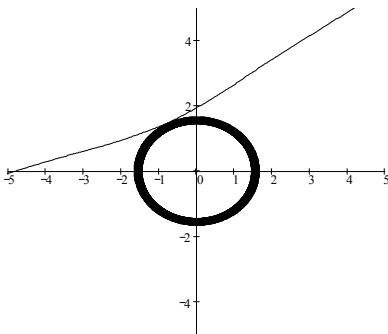inside the sphere is accordingly *P(r_1)=0.241*.

FIG. 8. A typical trajectory in the 2p-state. The circle is representing the sphere of the radius r_1.
Only the tangential point of the circle belongs to the trajectory. The coordinates in the plane of the
trajectory are measured in units of the Bohr radius *a*.

X. The 2p, m=1 state of the hydrogen atom

The knowledge of *K(r)* in the preceding section enables one to solve the equations of motion in the case of the m=1 and m=-1 states too. The differences are due to the different initial conditions.

Consider the m=1 state. The Lagrangian is the same as in the m=0 state,

$$L = \frac{1}{2} \cdot m \cdot \left(\frac{dr}{dt}\right)^2 + \frac{1}{2} \cdot m \cdot r^2 \cdot \left(\frac{d\phi}{dt}\right)^2 - U(r) \; , \tag{176}$$

but $\theta_0 = \frac{\pi}{4}$ or $\theta_0 = \frac{3 \cdot \pi}{4}$ for particles in the upper or lower half space, respectively. The trajectories have the same form of the time dependence and the same geometric shape as in the m=0 case, but the trajectories are now in planes making the angle $\theta_0 = \frac{\pi}{4}$ or $\theta_0 = \frac{3 \cdot \pi}{4}$ with the z-axis. The choice of this angle was explained in Sec. VI. The total angular momentum is set to be $\hbar \cdot \sqrt{2}$, the choice of the sign defining $\frac{d\phi}{dt}$ for a given total angular momentum. The angular momentum squared is then $2 \cdot \hbar^2$. In this m=1 trajectory the particle has always a positive angular frequency $\frac{d\phi}{dt} > 0$ such that $L_z = \hbar$, as was explained in Sec. VI. The particle is propagating always to the same direction on the trajectory. In m=0 state both directions of the particle motion existed on the same trajectory.
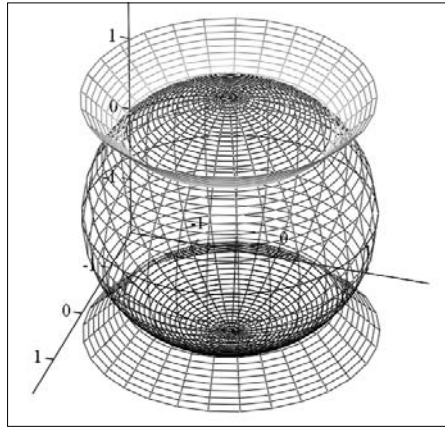
S,SS,SSS,SSSS

FIG. 9. The particle can have mechanical properties of a classical particle outside the sphere and outside the cones opening above and below the sphere. When localized outside those regions, the electron is at the same time found at some trajectory at some specific point of the trajectory. The particle trajectory is always in a plane, which is some tangent plane of the opening cones. These particlelike properties are given by the knowledge of the trajectories described earlier. The probability to find the particle on some of these trajectories is given by the wave function. The probability to find the electron inside the sphere is $P(r_1)=0.241$. The probability to find the particle inside the conic regions mentioned above is $P_c = 0.088$ and so the total probability is

$P(r_1)+P_c =0.329$. The probability to find the particle on some of the trajectories is slightly smaller than in the m=0 state being now $1- P(r_1)- P_c =0.671$.

XI. The linear harmonic oscillator in the polarized state

Consider the one-dimensional linear harmonic oscillator. The Schrödinger equation is

$$\hat{H} \cdot u(x) = E \cdot u(x) \ ,$$
(177)

where

$$\hat{H} = -\frac{\hbar^2}{2 \cdot m} \cdot \frac{d^2}{dx^2} + \frac{1}{2} \cdot k \cdot x^2 \ .$$
(178)

In order to facilitate the numerical computation, some specific choice of the parameters is necessary. That choice is

$$\hbar = 1 \ ,$$
(179)

$$m = \frac{1}{4} \ ,$$
(180)

and

$$k = 1 \ .$$
(181)

The wave function of the ground state is

$$u0(x) = \frac{1}{\sqrt{\sqrt{2 \cdot \pi}}} \cdot e^{-\frac{x^2}{4}} \ .$$
(182)

The wave function of the first exited state is

$$u0(x) = \frac{x}{\sqrt{\sqrt{2 \cdot \pi}}} \cdot e^{-\frac{x^2}{4}} \ .$$
(183)

The energy of the ground state is

$$E0 = 1 \ .$$
(184)

The energy of the first exited state is

$$E1 = 3 \ .$$
(185)

Writing $E0 = \dfrac{\hbar \cdot \omega}{2}$ and $E1 = \dfrac{3 \cdot \hbar \cdot \omega}{2}$, the angular frequency $\omega = 2$. The expectation values of the

kinetic energy in the ground state and in the first exited state, respectively, are $T0 = \dfrac{1}{2}$ and $T1 = \dfrac{3}{2}$.

The expectation values of the potential energy in the ground state and in the first exited state,

respectively, are in turn $V0 = \dfrac{1}{2}$ and $V1 = \dfrac{3}{2}$.

Let the oscillator be in a polarized state

$$\psi(x,t) = \cos(\alpha) \cdot u0(x) \cdot e^{-\frac{i \cdot E0 \cdot t}{\hbar}} + \sin(\alpha) \cdot u1(x) \cdot e^{-\frac{i \cdot E1 \cdot t}{\hbar}} . \tag{186}$$

Following the steps written down in Sec. VII, the expressions of the energy densities are obtained

first. Substituting the numerical values of $E0, E1, \omega$, and $\hbar$, the probability density can be written

as

$$\rho(x,t) = \left[\cos(\alpha)^2 + x^2 \cdot \sin(\alpha)^2 + 2 \cdot x \cdot \sin(\alpha) \cdot \cos(\alpha) \cdot \cos(2 \cdot t) \right] \cdot \frac{e^{-\frac{x^2}{2}}}{\sqrt{2 \cdot \pi}} . \tag{187}$$

The average total energy density $H_E(x,t)$ is

$$H_E(x,t) = \left[\cos(\alpha)^2 + 3 \cdot x^2 \cdot \sin(\alpha)^2 + 4 \cdot x \cdot \sin(\alpha) \cdot \cos(\alpha) \cdot \cos(2 \cdot t) \right] \cdot \frac{e^{-\frac{x^2}{2}}}{\sqrt{2 \cdot \pi}} . \tag{188}$$

The average kinetic energy density and the potential energy density respectively can be written as

$$H_K(x,t) = \left[\frac{1}{2} \cdot \cos(\alpha)^2 + \frac{3}{2} \cdot x^2 \cdot \sin(\alpha)^2 + 2 \cdot x \cdot \sin(\alpha) \cdot \cos(\alpha) \cdot \cos(2 \cdot t) \right] \cdot \frac{e^{-\frac{x^2}{2}}}{\sqrt{2 \cdot \pi}} , \tag{189}$$

$$H_U(x,t) = \left[\frac{1}{2} \cdot \cos(\alpha)^2 + \frac{3}{2} \cdot x^2 \cdot \sin(\alpha)^2 + 2 \cdot x \cdot \sin(\alpha) \cdot \cos(\alpha) \cdot \cos(2 \cdot t) \right] \cdot \frac{e^{-\frac{x^2}{2}}}{\sqrt{2 \cdot \pi}} , \tag{190}$$

and

$$H_E(x,t) = H_K(x,t) + H_U(x,t) . \tag{191}$$

The average total energy density is now being separated in two parts, the parts arising entirely either

from the kinetic energy or from the potential energy.

The potential energy density is written as

$$V(x,t) = \frac{1}{2} \cdot x^2 \cdot \rho(x,t) , \tag{192}$$

and the kinetic energy density can be found easily,

$$T(x,t) = H_E(x,t) - V(x,t) \ . \tag{193}$$

The expectation values of the total energy E, the kinetic energy $\langle\langle K \rangle\rangle$ and the potential energy $\langle\langle U \rangle\rangle$ of the classical system are identified to be

$$E = \cos(\alpha)^2 + 3 \cdot \sin(\alpha)^2 \ , \tag{194}$$

$$\langle\langle K \rangle\rangle = \frac{\cos(\alpha)^2 + 3 \cdot \sin(\alpha)^2}{2} \ , \tag{195}$$

$$\langle\langle U \rangle\rangle = \frac{\cos(\alpha)^2 + 3 \cdot \sin(\alpha)^2}{2} \ . \tag{196}$$

The relative potential energy density *Vden(x,t)* and the relative kinetic energy density *Tden(x,t)= -Vden(x,t)* can be obtained as was explained in Sec. VII. The graph of Fig. 10 is displaying the relative potential energy density, when $\alpha = \dfrac{\pi}{4}$ and $t = \dfrac{\pi}{4} \cdot 0.99$.
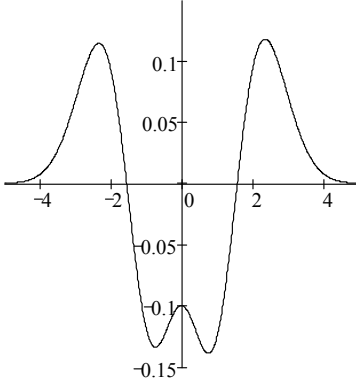

FIG. 10. The relative potential energy density *Vden* plotted against *x*, when $\alpha = \pi/4$ and *t=0.99·π/4*.

In order to calculate the potential energy, the same algorithm, which was developed in Sec. VIII in the case of the ground state of the hydrogen atom, can be applied in this one-dimensional case. That algorithm requires the inverse function of the function $\varepsilon = Vden(x,t,\alpha)$. Denoting by

$$x = g(\varepsilon,t,\alpha,j) \tag{197}$$

the jth branch of the inverse function such, that for instance $x = g(\varepsilon,t,\alpha,0)$ is the inverse function to be used for values of x in the interval $[-\infty, extr1]$, where $extr1$ is denoting the x-coordinate of the extremum of the function $\varepsilon = Vden(x,t,\alpha)$ with the smallest value of x. The graph in Fig. 11 is displaying the inverse function for all values of x. In that graph $extr1$ denotes the x-coordinate of the extremum lowest in the graph. Denote by $zero1$ the zero-point of the function $Vden(x,t,\alpha)$ such that the x-coordinate is the smallest. The x-coordinate of the zero-point of the function $Vden(x,t,\alpha)$ lowest in the graph is denoted by $zero1$ in the graph of Fig. 11.
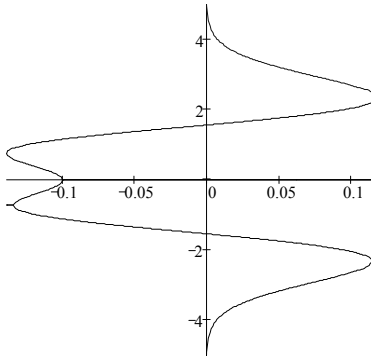

FIG. 11. The inverse function of the relative potential energy density $\varepsilon = Vden(x,t,\alpha)$, when $\alpha = \pi/4$ and $t=0.99\cdot \pi/4$.

The potential energy, for instance in the interval $[-\infty, zero1]$, will be obtained first by calculating the potential energy denoted now by $V\varepsilon$ as a function of the relative potential energy density ε. Applying the algorithm developed in Sec. VIII one obtains for $-\infty < x < zero1$,

$$V\varepsilon(\varepsilon,t,\alpha) = \varepsilon \cdot (g(\varepsilon,t,\alpha,,1) - g(\varepsilon,t,\alpha,0)) - \int_0^\varepsilon (g(\varepsilon,t,\alpha,,1) - g(\varepsilon,t,\alpha,0)) \cdot d\varepsilon \ . \tag{198}$$

The potential energy function, denoted now by $V\varepsilon\varepsilon(x,t,\alpha)$, is then obtained as a function of x by substituting $\varepsilon = Vden(x,t,\alpha)$ into the expression of $V\varepsilon(\varepsilon,t,\alpha)$ yielding

$$V\varepsilon\varepsilon(x,t,\alpha) = V\varepsilon(Vden(x,t,\alpha),t,\alpha) \ , when \ -\infty < x < zero1 \tag{199}$$

This potential energy function is now the primitive of the indefinite integral vanishing at the boundary of the system in the infinity. The constants of the integration are to be determined next.

The following graph Fig. 12 is the potential energy function $V_{\varepsilon\varepsilon}(x,t,\alpha)$, when the constant of the integration $C2(t)$ defined in Sec. VII is identically zero.
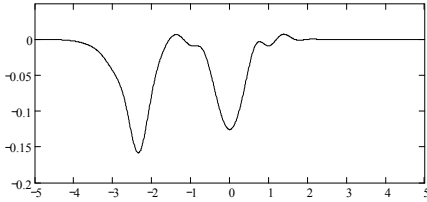

FIG. 12. The vertical axis: the potential energy of the particle as a function of the particle coordinate x. The graph is obtained by setting the constant of the integration $C2(t)=0$. The graph is describing the situation $\alpha = \pi/4$ and $t=0.99\cdot\pi/4$.

Following the procedure developed in Sec. VII, the equation of the motion is to be solved next. The boundary conditions are such that the kinetic energy at the infinity must be

$$\langle\langle K\rangle\rangle = \frac{\cos(\alpha)^2 + 3\cdot\sin(\alpha)^2}{2} \quad . \tag{200}$$

In order to solve the equation of motion, the force acting on the particle must be determined,

$$F_{\varepsilon}(x,t,\alpha) = -\frac{dV_{\varepsilon\varepsilon}(x,t,\alpha)}{dx} \quad . \tag{201}$$

This force is being displayed in Fig 13. As can be seen, the force is zero at large distances from the origin. The equations of motion have been solved for a positive velocity of the particle, with application of the boundary condition in the infinity. The results are shown in Figs. 14, 15, and 16.
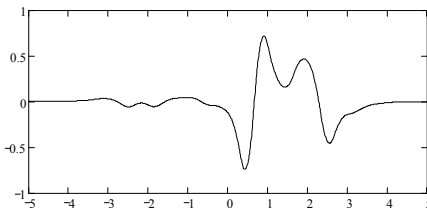

FIG. 13. The force acting on the particle as a function of x. The graph is obtained, when $\alpha = \pi/4$ and $t=0.99\cdot\pi/4$.
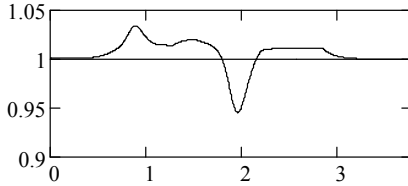
FIG. 14. The kinetic energy plotted as a function of time on the particle trajectory with positive velocity, when $\alpha = \pi/4$. The horizontal line is the expectation value of the kinetic energy. Because the constants of integration *C1(t)* and *C2(t)* are known now, the potential energy may be determined. See the graph of Fig. 15 for the potential energy.
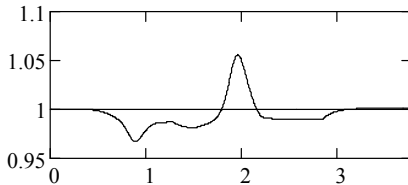

FIG. 15. The potential energy plotted as a function of time on the particle trajectory with positive velocity, when $\alpha = \pi/4$. The horizontal line is the expectation value of the potential energy.

The kinetic energy

$$E_K(t) = \frac{1}{2} \cdot m \cdot \left(\frac{dx(t)}{dt} \right)^2 \ , \tag{202}$$

is being displayed in Fig. 14 as a function of the position *x* on the particle trajectory. The potential energy is shown in Fig.15 as a function of time on the particle trajectory.

In Fig. 16 the velocity difference of the particle and a fictitious particle is shown. The fictitious particle moves with the same asymptotic velocity the particle has on the boundary of the system. The graph has been obtained as a function of the position *x*. The boundary condition

$$\langle\langle K \rangle\rangle = \frac{\cos(\alpha)^2 + 3 \cdot \sin(\alpha)^2}{2} \ , \tag{203}$$

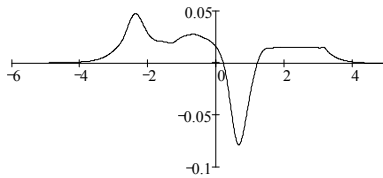is satisfied, as can be seen from the graph.

FIG. 16. The vertical axis: the velocity difference of the particle and a fictitious particle . The fictitious particle is moving with the same positive asymptotic velocity the particle has on the boundaries of the system.The graph has been obtained as a function of x, when $\alpha = \pi/4$.

The graphs seen in Fig. 17 are in fact interesting. The graph denoted by xin is describing the particle trajectory obtained in a state $\psi(x,t)$.The particle is propagating with negative velocity on this trajectory. The graph denoted by $x\Delta t$ t is describing the particle trajectory, which would be obtained in a state $\psi(x,t+\Delta t)$, when $\Delta t = \dfrac{\pi}{6}$. The particle is propagating with positive velocity on that trajectory. The trajectories intersect, when $x=0.314$. At $x=0.314$ the particle trajectory has in a state $\psi(x,t)$ the velocity $vin=-2.761$. Suppose that velocity would be instantly changed at that position to be $v\Delta t = 2.807$, which is the velocity of the particle going to the positive direction in the trajectory xin at that point $x=0.314$, where the trajectories intersect. Two interesting questions arise. Would the particle get delocalized into a state, which has the properties of the state $\psi(x,t+\Delta t)$? If that will happen, what kind of circumstances that would require?
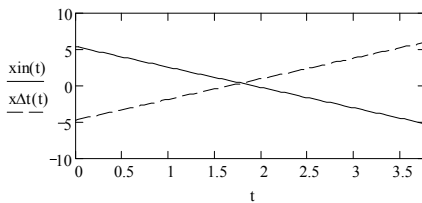

FIG. 17. The graph denoted by $xin(t)$, the solid line, is describing the particle trajectory obtained in the state $\psi(x,t)$ and the particle is propagating with negative velocity as a function of time. The graph denoted by $x\Delta t$ (t), the dashed line, is describing the particle trajectory that would be obtained in the state $\psi(x,t+\Delta t)$ and the particle is propagating with positive velocity.

XII. The nucleus ^{17}O

The nucleus ^{17}O will be considered as the next example. The valence neutron is in the $1d_{5/2}$ shell. The radial wave function is obtained using the Woods-Saxon shell model potential

$$U = V \cdot g(r) + V_{ls} \cdot (\boldsymbol{l} \cdot \boldsymbol{s}) \cdot r_0^2 \cdot \frac{1}{r} \cdot \frac{dg(r)}{dr} \tag{203}$$

where $V_{ls} = -0.44 \cdot V$ and V is left as a free parameter to be deduced from the experimental neutron separation energy -4.14 MeV. This choice will give $V = -51.7$ MeV. The function $g(r)$ is given by

$$g(r) = \left[1 + \exp((r-R)/a)\right]^{-1} \tag{204}$$

where $R = r_0 \cdot A^{1/3}$, $r_0 = 1.25$ fm , $a = 0.65$ fm. See e.g. [1] for the parameterisation.

Similar calculation as in Sec. **X** yields the kinetic energy and so the speed as a function of r, the nuclear radius. See Fig. 18, Fig.19 below. The radial kinetic energy becomes negative at distances less than $rlimit = 2.675$ fm. The particle cannot get localized at distances closer to the origin because of the centrifugal barrier.

The velocity of the neutron in the nucleus can be measured directly in the framework of the direct knockout reaction $^{17}O(p,np)^{16}O$. Theoretically the easiest geometry is obtained, when the projectile proton is measured on the beam axes in the forward direction and the knocked out neutron is observed perpendicular to the beam at polar angle 90 degrees. The conservation of the energy and momentum give

$$\begin{aligned} m_p \cdot v_{ip} + m_n \cdot v_{in} \cdot \cos(\theta) &= m_p \cdot v_{fp} \\ m_n \cdot v_{in} \cdot \sin(\theta) &= m_n \cdot v_{fn} \\ \frac{1}{2} \cdot m_p \cdot v_{ip}^2 + E_n &= \frac{1}{2} \cdot m_p \cdot v_{fp}^2 + \frac{1}{2} \cdot m_n \cdot v_{fn}^2 \end{aligned} \tag{205}$$

Here θ is the polar angle of the initial neutron velocity and v_{in} is initial speed of the neutron before the collision. Similarly v_{fn}, v_{ip}, v_{fp} denote the final speed of the neutron, the initial speed of the projectile proton and the final speed of the projectile proton, respectively. The neutron and proton masses are denoted by m_n and m_p, respectively. The neutron separation energy is E_n. The speeds v_{fp} and v_{fp} are measured in coincidence, the condition of the coincidence being the equations (205). The angle θ becomes determined from these equations. The next step is to write down the conservation of the angular momentum, while the incoming proton and the outgoing proton carry no angular momentum. Let α denote the polar angle of the radius vector of the initial neutron. The conservation of the angular momentum implies then

$$m_n \cdot v_{in} \cdot r \cdot \sin(\theta - \alpha) = m_n \cdot v_{fn} \cdot r \cdot \cos(\alpha)$$
$$m_n \cdot v_{fn} \cdot r \cdot \cos(\alpha) = \hbar \cdot \sqrt{l \cdot (l+1)}$$

(206)

The position of the initial neutron becomes defined through the equations (205). This experiment will evidently determine v_{in} as a function of r to be compared with the theoretical prediction Fig. 18 below.
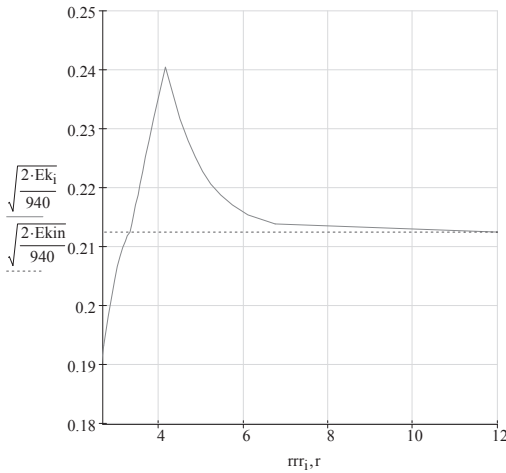

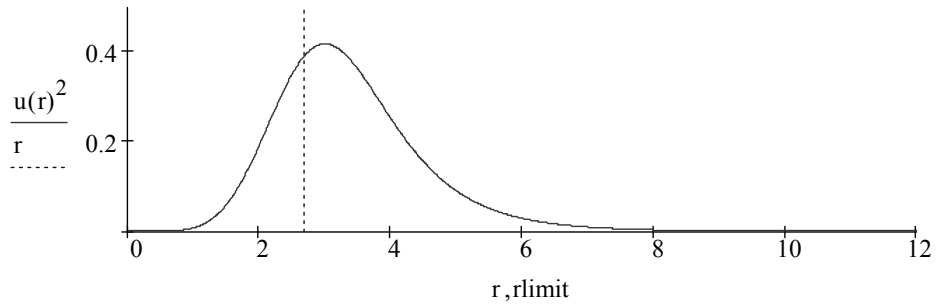FIG. 18. The speed of the valence neutron in units of the speed of light as a function of r in fm.

FIG. 19. The radial probability density, *r* in fm. The limiting radius *rlimit*, the dashed line.

XIII. Conclusions

The present approach gives the proof that a bijection exists between two systems. The other system is given by the Schrödinger equation in the form of the wave mechanics and the other system obeys the Newton mechanics. Particlelike properties are known to exist in quantum systems. On the other hand, the uniqueness of the classical particle motion obtained from the given equation of the Hamilton density was proven in this paper. Therefore, due to this uniqueness, if particlelike properties are found in a quantum mechanical state, those are most probably given by the equation of the Hamilton density obtained from the Schrödinger equation. For example, a knockout reaction of the particle with by a direct impact could probably reveal those particlelike properties. In any case, we should be able to enhance the information that is obtained from the experiments in comparison with the information obtained from the wave mechanics only. How the observables in the wave mechanical system and in the equivalent classical system are correlated, cannot be concluded exactly without experiments. Some interpretations of this correlation were presented in this work using a working hypothesis. In brief, the working hypothesis was that beneath of the usual quantum mechanical description of the system in the form of the wave mechanics, the system has predictable particlelike properties. These particlelike properties can be predicted by the particle trajectories, which may fill either the whole space-time or only some predictable regions of the space-time. The probability to find the particle is always given by the wave function, no matter the particle is found on some trajectory or not. For this reason the particle does not actually propagate along a trajectory, but the trajectory and the location of the particle on the trajectory are stochastic variables.

References

[1]   P.Haapakoski. Mod. Phys Lett. A, Vol. 2, No 6(1987)359-366

Appendix

A. Mechanical system in an external field

1. The description of the system

Suppose we are given for a certain particle of mass *m* in the interval *–a<x<a* the average energy density

$$H_E(x,t) = H_K(x,t) + H_U(x,t) \ ,$$

<div align="right">A1</div>

where

$$H_K(x,t) = \frac{k \cdot a}{8} + \cos^2\left(\frac{x \cdot \pi}{2 \cdot a}\right) \cdot \sin(\omega \cdot t) - \frac{1}{2} \cdot \sin(\omega \cdot t) \ ,$$

<div align="right">A2</div>

$$H_U(x,t) = \frac{k \cdot a}{8} + 2 \cdot \sin^2\left(\frac{x \cdot \pi}{a}\right) \cdot \cos(\omega \cdot t) - \cos(\omega \cdot t) \ .$$

<div align="right">A3</div>

Here $H_U(x,t)$ is the contribution of the potential energy to the average energy density and $H_K(x,t)$ the contribution of the kinetic energy respectively. The total energy *E*, the expectation values of the kinetic energy $\langle\langle K \rangle\rangle$, and the potential energy $\langle\langle U \rangle\rangle$, respectively, are given below:

$$E = \int_{-a}^{a} H_E(x,t) \cdot dx = \frac{k \cdot a^2}{2} \ ,$$

<div align="right">A4</div>

$$\langle\langle K \rangle\rangle = \int_{-a}^{a} H_K(x,t) \cdot dx = \frac{k \cdot a^2}{4}$$

<div align="right">A5</div>

$$\langle\langle U \rangle\rangle = \int_{-a}^{a} H_U(x,t) \cdot dx = \frac{k \cdot a^2}{4}$$

<div align="right">A6</div>

$$E = \langle\langle K \rangle\rangle + \langle\langle U \rangle\rangle$$

<div align="right">A7</div>

Given the kinetic energy density,

$$T(x,t) = \begin{cases} -\dfrac{k \cdot x}{2} + \dfrac{k \cdot a}{8} + \cos^2\left(\dfrac{x \cdot \pi}{2 \cdot a}\right) \cdot \sin(\omega \cdot t) - \dfrac{1}{2} \cdot \sin(\omega \cdot t) & when \ \ x \geq 0 \\[3mm] \dfrac{k \cdot x}{2} + \dfrac{k \cdot a}{8} + \cos^2\left(\dfrac{x \cdot \pi}{2 \cdot a}\right) \cdot \sin(\omega \cdot t) - \dfrac{1}{2} \cdot \sin(\omega \cdot t) & when \ \ x < 0 \end{cases} \ ,$$

<div align="right">A8</div>

and the potential energy density,

$$V(x,t) = \begin{cases} \left(\dfrac{k \cdot x}{2} + \dfrac{k \cdot a}{8} + \cos^2\left(\dfrac{x \cdot \pi}{2 \cdot a}\right) \right) \cdot \sin(\omega \cdot t) - \dfrac{1}{2} \cdot \sin(\omega \cdot t) \quad when \quad x \geq 0 \\ \left(-\dfrac{k \cdot x}{2} + \dfrac{k \cdot a}{8} + \cos^2\left(\dfrac{x \cdot \pi}{2 \cdot a}\right) \right) \cdot \sin(\omega \cdot t) - \dfrac{1}{2} \cdot \sin(\omega \cdot t) \quad when \quad x < 0 \end{cases} , \qquad \text{A9}$$

the equation of the Hamiltonian density can be written as:

$$T(x,t) + V(x,t) = H_E(x,t) \ . \qquad\qquad \text{A10}$$

This system is obviously such, that the conditions of Sec. III for an equation of the Hamiltonian density of a classical particle obeying the laws of the Newton mechanics are fulfilled [see Eqs. (28)-(33)]. Classical particle motion can be obtained as in Sec. III.

The boundary conditions for the motion are obviously such, that the kinetic energy must be zero at the end points of the interval.

2. The solution of the particle motion

The next step in solving the physical system is to define the relative energy densities as

$$Vden(x,t) = V(x,t) - H_U(x,t), \qquad\qquad \text{A11}$$

and

$$Tden(x,t) = T(x,t) - H_K(x,t) \qquad\qquad \text{A12}$$

The two important equations covering the relative energy densities are obtained as

$$Vden(x,t) + Tden(x,t) = 0, \qquad\qquad \text{A13}$$

$$Tden(x,t) = -Vden(x,t) \ . \qquad\qquad \text{A14}$$

These equations concerning *Tden* and *Vden* contain the same information as the equation

$$T(x,t) + V(x,t) = H_E(x,t) \ , \qquad\qquad \text{A15}$$

when applied together with the Eqs. (A4)-(A7).

The next thing to do is to form the indefinite integral of the equation covering the relative energy densities, while the differential element of the integration is a volume element (segment length element in this one dimensional case) such, that the primitives are zero at the boundaries of the system. This volume element will be defined by the equidensity surfaces of the potential energy

density *Vden*. These are also the equidensity surfaces of *Tden* as well. In order to construct these surfaces the inverse function of the potential energy density *Vden* is required. Denoting

$$\varepsilon_U = Vden(x,t) \qquad\qquad\qquad\qquad\qquad \text{A16}$$

the relative potential energy density can be written

$$\varepsilon_U = \begin{cases} \dfrac{k \cdot x}{2} & when \quad x \geq 0 \\ \dfrac{-k \cdot x}{2} & when \quad x < 0 \end{cases}. \qquad\qquad\qquad\qquad \text{A17}$$

As can be seen, in this application the relative potential energy density becomes independent of time. The inverse function is of course independent of time as well and can be written as

$$x = \begin{cases} \dfrac{2 \cdot \varepsilon_U}{k} & when \quad x \geq 0 \\ \dfrac{-2 \cdot \varepsilon_U}{k} & when \quad x < 0 \end{cases}. \qquad\qquad\qquad\qquad \text{A18}$$

Denoting

$$f(\varepsilon_U,0) = \frac{-2 \cdot \varepsilon_U}{k}, \qquad\qquad\qquad\qquad\qquad \text{A19}$$

and

$$f(\varepsilon_U,1) = \frac{2 \cdot \varepsilon_U}{k}, \qquad\qquad\qquad\qquad\qquad \text{A20}$$

the inverse function of the function *Vden* is ready to use. Consider a closed surface $S(\Omega)$ *)* such that the function *Vden* is a constant on this surface, the volume enclosed by the surface is denoted by Ω. Consider then another surface infinitesimally close to the earlier surface such that the function *Vden* is a constant on this surface. Consider the volume of this surface and denote the volume enclosed by this surface by $\Omega + d\Omega$. Then the potential energy difference between the two surfaces is

$$dU = Vden(x) \cdot d\Omega \qquad\qquad\qquad\qquad\qquad \text{A21}$$

In this example the volume is a segment length and the infinitesimal volume difference is the infinitesimal segment length difference. The surface $S(\Omega)$ is in this one dimensional example represented by the end points of the segment.

When the relative potential energy density is ε_U, the end points of the segment in question are at distance $f(\varepsilon_U,1) - f(\varepsilon_U,0)$ from each other. The infinitesimal length difference $d\Omega$ can be computed as a function of ε_U as

$$d\Omega = \left(f'(\varepsilon_U,1) - f'(\varepsilon_U,0)\right) \cdot d\varepsilon_U. \qquad\qquad\qquad\qquad \text{A22}$$

Substituting $f(\varepsilon_U,0)$ from Eq. (A19) and $f(\varepsilon_U,1)$ from Eq. (A29) into Eq. (A22) yields

$$d\Omega = \left(\frac{2}{k} - \frac{-2}{k}\right) \cdot d\varepsilon_U,$$ A23

$$d\Omega = \frac{4}{k} \cdot d\varepsilon_U .$$ A24

The next thing to do, is to carry out the indefinite integral of the equation

$$Tden(x) + Vden(x) = 0,$$ A25

$$\left(\int Tden(x) \cdot d\Omega + C1\right) + \left(\int Vden(x) \cdot d\Omega + C2\right) = C3.$$ A26

Because in this application *Tden* and *Vden* are independent of time the constants of integration are also independent of time. The two constants of integration *C1* and *C2* are written separately just for convenience. The second expression in the brackets is to be considered as a potential energy. Likewise the first bracketed expression is the kinetic energy. Then *C3* is the total energy and it is set to be *C3=E*.

Denoting by *U* the potential energy of the particle and substituting the expressions (A27) and (A28) into the expression of the potential energy, which is given by Eq. (A26), yields the expression of $U(\varepsilon_U)$ given in Eq. (A29) below. Let

$$Vden(x) = \varepsilon_U ,$$ A27

and

$$d\Omega = \frac{4}{k} \cdot d\varepsilon_U ,$$ A28

then

$$U(\varepsilon_U) = \int_0^{\varepsilon_U} \varepsilon_U \cdot \frac{4}{k} \cdot d\varepsilon_U + C2 \quad ,$$ A29

yielding

$$U(\varepsilon_U) = \frac{2 \cdot \varepsilon_U^2}{k} + C2 .$$ A30

Substituting now for ε_U in this equation (A.30) the expression of ε_U of Eq. (A17) results

$$U(x) = \frac{k \cdot x^2}{2} + C2 .$$ A31

Consider the particle inside the interval $-a<x<a$ with the total energy E and subject to the boundary conditions $K(-a)=K(a)=0$. The kinetic energy is of course $K(x)=E-U(x)$ and the substitution of $U(x)$ into this expression yields

$$K(x) = E - \frac{k \cdot x^2}{2} - C2 \ ,$$
A32

$$K(x) = \frac{k \cdot a^2}{2} - \frac{k \cdot x^2}{2} - C2$$
A33

Because of the boundary conditions $K(-a)=K(a)=0$ the constant of integration $C2=0$. The final result is that the potential energy of the particle is

$$U(x) = \frac{k \cdot x^2}{2} \ ,$$
A34

and the kinetic energy is

$$K(x) = \frac{k \cdot a^2}{2} - \frac{k \cdot x^2}{2} \ .$$
A35

A fairly simple system was embedded in these fields given at the beginning of this section, a classical particle motion in the harmonic oscillator potential.

B. The classical harmonic oscillator

Let the oscillator potential energy be

$$U(x) = \frac{k \cdot x^2}{2} \ .$$
A36

The derivation of the potential energy density will involve finding first the closed surfaces $S(\Omega)$ with constant potential energy on the surface. Then the potential energy difference between two surfaces differing only infinitesimally from each other would be

$$dU = U(\Omega + d\Omega) - U(\Omega) \ .$$
A37

On the other hand,

$$dU = Vden(\Omega) \cdot d\Omega \ ,$$
A38

Because of Eq. (A38) the relative potential energy density can be obtained as the derivative

$$Vden(\Omega) = \frac{dU}{d\Omega} \quad . \tag{A39}$$

In this one dimensional case the closed surface will be presented with the end points of a segment and the differential element $d\Omega$ will be presented by the infinitesimal change in the length of this segment. In order to estimate this change, the inverse of the potential energy $U(x) = \frac{k \cdot x^2}{2}$ can be used. That inverse function is

$$x = \begin{cases} \sqrt{\dfrac{2 \cdot U}{k}} & when \quad x \geq 0 \\ -\sqrt{\dfrac{2 \cdot U}{k}} & when \quad x < 0 \end{cases} \quad . \tag{A40}$$

Denoting in Eq. (A40) above

$$g(U,0) = -\sqrt{\frac{2 \cdot U}{k}} \quad , \tag{A41}$$

and

$$g(U,1) = \sqrt{\frac{2 \cdot U}{k}} \quad , \tag{A42}$$

the infinitesimal change of the length $g(U,1) - g(U,0)$ of the segment can be written as

$$d\Omega = (g'(U,1) - g'(U,0)) \cdot dU \tag{A43}$$

The derivative $\dfrac{dU}{d\Omega}$ is found from Eq. (A43) as

$$\frac{dU}{d\Omega} = \sqrt{\frac{k}{2}} \cdot \sqrt{U} \quad , \tag{A44}$$

and consequently, the relative potential energy density (A39) can be written as a function of U as

$$Vden(U) = \sqrt{\frac{k}{2}} \cdot \sqrt{U} \tag{A45}$$

Substituting now for U in Eq. (A45) its expression in terms of x, given by Eq. (A36), will yield the relative potential energy density as a function of x. This relative potential energy density is independent of the actual motion, independent of the total energy and independent of the initial conditions of the motion.

$$Vden(x) = \begin{cases} \dfrac{k \cdot x}{2} & when \quad x \geq 0 \\ \dfrac{-k \cdot x}{2} & when \quad x > 0 \end{cases} \quad . \tag{A46}$$

Because

$$Tden(x) + Vden(x) = 0 \ ,$$ A47

the relative kinetic energy density is obtained

$$Tden(x) = -Vden(x)$$ A48

More explicitly this can be written

$$Tden(x) = \begin{cases} \dfrac{-k \cdot x}{2} & when \quad x \geq 0 \\ \dfrac{k \cdot x}{2} & when \quad x < 0 \end{cases}$$ A49

The next step is to obtain the potential energy density and the kinetic energy density, $V(x)$ and $T(x)$, respectively. For that purpose the knowledge of the actual motion is required. The motion is assumed to happen in the interval $-a<x<a$ such, that $K(-a)=K(a)=0$ and $E = \dfrac{k \cdot a^2}{2}$

Let the average total energy density $H_E(x)$ be a constant and

$$H_E(x) = \frac{E}{\Omega tot} = \frac{E}{2 \cdot a} = \frac{k \cdot a}{4} \ .$$ A50

The total energy is

$$E = \langle\langle K \rangle\rangle + \langle\langle U \rangle\rangle \ .$$ A51

For a classical harmonic oscillator a half of the total energy E is due to the potential energy and the other half from the kinetic energy. The expectation values of the classical motion are

$$\langle\langle K \rangle\rangle = \frac{k \cdot a^2}{4} \ ,$$ A52

$$\langle\langle U \rangle\rangle = \frac{k \cdot a^2}{4} \ .$$ A53

The average kinetic energy density and the average potential energy density can be written as

$$H_K(x) = \frac{k \cdot a}{8} \ ,$$ A54

$$H_U(x) = \frac{k \cdot a}{8} \ .$$ A55

These numbers are just the expectation values (time averages) of the potential energy and the kinetic energy divided by the volume (the length of the interval, which is $2a$). Adding these numbers into the equation binding *Tden* and *Vden* yields

$$(Tden(x) + H_K(x)) + (Vden(x) + H_U(x)) = H_E(x) \ .$$ A56

The kinetic energy density $T(x)$ and the potential energy density $V(x)$ of the actual motion are identified as the bracketed expressions in Eq. (A56), yielding

$$V(x) = \begin{cases} \dfrac{k \cdot x}{2} + \dfrac{k \cdot a}{8} & when \quad x \geq 0 \\ \dfrac{-k \cdot x}{2} + \dfrac{k \cdot a}{8} & when \quad x < 0 \end{cases} \text{,} \qquad \text{A57}$$

$$T(x) = \begin{cases} \dfrac{-k \cdot x}{2} + \dfrac{k \cdot a}{8} & when \quad x \geq 0 \\ \dfrac{k \cdot x}{2} + \dfrac{k \cdot a}{8} & when \quad x < 0 \end{cases} \text{.} \qquad \text{A58}$$

The equation of the Hamiltonian density takes finally the form

$$T(x) + V(x) = H_E(x) \quad , \qquad \text{A59}$$

where

$$H_E(x) = H_K(x) + H_U(x) \quad , \qquad \text{A60}$$

and $T(x)$, $V(x)$, $H_K(x)$, and $H_U(x)$ are given by Eqs. (A58), (A57), (A54), and (A55), respectively.

Here is an example, how a classical particle motion in a conservative system can be interpreted in terms of the equation of the Hamiltonian density: The kinetic energy density, the potential energy density, and the total energy density such, that the total energy is E and the expectation values (the time averages) of the kinetic energy and the potential energy are $\langle\langle K \rangle\rangle$ and $\langle\langle U \rangle\rangle$, respectively. The former example considered the same oscillator and the same motion in fact, in such a medium, that the motion of the oscillator did not get distorted at all.