Chapter 10

Non-Hamiltonian Quantization Method

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10.1 Introduction

Even in its early stages, Quantum Mechanics was already involved with the problem of non-Hamiltonian systems, mainly related with dissipation [1,2]. The approaches adopted to deal with these situations separate into two distinct strategies:

- some [1] tried a more direct approach by proceeding to the quantization of an open physical system assuming a dissipative velocity dependent force of the type $-kv$. The difficulty here is the obvious departure from the usual Hamiltonian formalism that will hinder quantization in its usual form. The usual approach, then, is to propose reformulations of the Hamiltonian formalism to embrace dissipation [3], for instance, and provide (possibly) a bridge to Quantum Mechanics using the known quantization approach. Thus, one changes the underlying classical structure to keep (at least to a large extent) the quantization method. This, however, has shown to be exceedingly difficult to accomplish and also pervaded by arbitrariness[4];
- others [2] preferred to think about the problem as being an isolated physical system with two subsystems, one of them taking energy from the other because of its large number of accessible states. This kind of approach assumes an overall isolated system with one of the subsystems acting as a heat bath and has attracted additional attention [5] in more recent years. It is generally criticized for its need to model the heat bath (generally using harmonic oscillators), while one would possibly desire an approach in which the specific and detailed structure of the bath could be disregarded - a phenomenological approach in which these details are embedded into the phenomenological constant.

That being said, it seems to be highly desirable to have a quantization method that does not depend upon the Hamiltonian formalism and is still capable of arriving at the Schrödinger equation for all usual (non dissipative) physical situations. If one has such a method, then it can be easily extended to find a modified Schrödinger equation that takes into account dissipative effects. It will leave Hamiltonian Classical Physics as it is, it will not assume a heat reservoir as part of the overall system, and the focus would be the quantization process itself.

This has already been done [6] and, as we will show here, provided a modified (generalized) Schrödinger equation [7] that gives the usual one for Hamiltonian situations. The modified Schrödinger equation that emerged is much more difficult to solve analytically. However, such solutions can help one figuring out the very physics of the process of dissipation in Quantum Mechanics.

The present paper goal is to produce such a solution for the 'free' (with dissipation, of course) wave-packet movement. We will show that the quantization method gives rise to a different kind of behavior, compared to the usual ones made by assuming a complex potential, which gives, for its imaginary part, *the dissipation of the involved quantum mechanical state* and the promotion of another state - giving, thus, a description of metastability.

To accomplish that in a sound way, we will present the derivation in section 10.2, which departs from only *two axioms*. In section 10.3, as a means to establish the soundness of the formal *usual* quantization approach, we present the problem of quantization in general coordinates, tackled in very different ways from what is generally done. The problem shows itself very involved, despite algebraically straightforward, and should increase the confidence of the reader on the quantization method. In section 10.4, we begin to show that the quantization method here proposed has other consequences; one of them is the possibility of mathematically deriving the Bohr-Sommerfeld rules. Section 10.5 shows the close connection of the present quantization method (so far developed only for Hamiltonian systems) with Feynman's path integral approach. This is important, since it unravels the interpretation of some assumptions in our derivation process (development up to second order of a parameter, as will be presented). Finally, as a means to show the far reaching consequences of the quantization method, we show, in section 10.6 that this quantization method is connected to the Central Limit Theorem. At this point, we assume that the reader is confident enough regarding the usual quantization method (for Hamiltonian systems) and we proceed to develop the strategy for non-Hamiltonian systems in section 10.7. The approach is mathematically quite simple and direct and gives an easy enough interpretation of the problem within quantum mechanics. In section 10.8 we begin our presentation of the free wave-packet problem, now in the presence of dissipation of the type $-kv$, where v is the velocity and k is a phenomenological constant. We then show that the effect of the dissipation is to halt the movement of the packet. In section 10.9 we present our conclusions.

10.2 Characteristic Function Derivation

We begin our axiomatization of Quantum Mechanics by presenting the axioms and showing that they allow us to *mathematically derive* the Schrödinger equation[6].

Axiom 1 *The characteristic function of the phase-space probability density function*

$F(q,p;t)$, defined by

$$Z\left(q,\delta q;t\right)=\int_{-\infty}^{+\infty}F\left(q,p;t\right)e^{ip\delta q/\ell}dp, \tag{10.1}$$

where ℓ is a universal parameter with dimensions of angular momentum, is such that it can be written as

$$Z\left(q,\delta q;t\right)=\psi^*\left(q-\frac{\delta q}{2};t\right)\psi\left(q+\frac{\delta q}{2};t\right), \tag{10.2}$$

and should be expanded up to second order in the parameter δq.

Axiom 2 *For an isolated system, the joint phase-space probability density function related to any Quantum Mechanical phenomenon obeys the Fourier transformed Liouville equation*

$$\int\exp\left(i\frac{p\delta q}{\ell}\right)\frac{dF\left(q,p;t\right)}{dt}=0; \tag{10.3}$$

The derivative in (10.3) may be written as

$$\frac{dF\left(q,p;t\right)}{dt}=\frac{\partial F}{\partial t}+\frac{p}{m}\frac{\partial F}{\partial q}-\frac{\partial V}{\partial q}\frac{\partial F}{\partial p}=0\,, \tag{10.4}$$

where it is already assumed that the underlying forces may be written as the gradient of a potential function. We now apply transformation (10.1) to this last equation and use the fact that $F\left(q,p;t\right)$ is a probability density function to put

$$\left\{F\left(q,p;t\right)e^{ip\delta q/\ell}\right\}_{p=-\infty}^{p=+\infty}=0\,, \tag{10.5}$$

to arrive at the equation

$$-\frac{\ell^2}{m}\frac{\partial^2 Z}{\partial q\partial\left(\delta q\right)}+\delta q\frac{\partial V}{\partial q}Z=i\ell\frac{\partial Z}{\partial t}, \tag{10.6}$$

that is the differential equation for the characteristic function $Z\left(q,\delta q;t\right)$.

We can write the function $Z\left(q,\delta q;t\right)$ in terms of the functions $\psi\left(q;t\right)$ presented in (10.2) *and expand it up to second order* in δq. Thus, putting

$$\psi\left(q;t\right)=R\left(q;t\right)e^{iS(q;t)/\ell}, \tag{10.7}$$

since $\psi\left(q;t\right)$ is, in general, a complex function, we get, after expanding it up to second order in δq, the result

$$Z\left(q,\delta q;t\right)=\left\{R^2+\left(\frac{\delta q}{2}\right)^2\left[R\left(q;t\right)\frac{\partial^2 R}{\partial q^2}-\left(\frac{\partial R}{\partial q}\right)^2\right]\right\}\times\exp\left(\frac{i\delta q}{\ell}\frac{\partial S}{\partial q}\right). \tag{10.8}$$

Now we put expression (10.8) into (10.6) and separate the real and imaginary terms to find equations

$$\frac{\partial R^2}{\partial t}+\frac{\partial}{\partial q}\left[\frac{R(q;t)^2}{m}\frac{\partial S\left(q,t\right)}{\partial q}\right]=0 \tag{10.9}$$

and

$$i\frac{\delta q}{\ell}\frac{\partial}{\partial q}\left[\frac{\partial S}{\partial t}+\frac{1}{2m}\left(\frac{\partial S}{\partial q}\right)^2+V\left(q\right)-\frac{\ell^2}{2mR}\frac{\partial^2 R}{\partial q^2}\right]=0. \tag{10.10}$$

The first equation may be identified as a continuity equation, as the result of a semantic inheritance related to the interpretation of the axioms' symbols. Indeed, since we have written the characteristic function as in (10.2) and also put ψ as in (10.7), we immediately find that

$$R\left(q;t\right)^2 = \lim_{\delta q \to 0} Z\left(q,\delta q;t\right) = \psi^*\left(q;t\right)\psi\left(q;t\right) = \int_{-\infty}^{+\infty} F\left(q,p;t\right)dp\,, \tag{10.11}$$

which must be a probability density function defined upon configuration space, *since* $F\left(q,p;t\right)$ is a probability density function defined upon phase space—this means that $\psi\left(q;t\right)$ *must* be a probability amplitude, an interpretation inherited from the axioms. It is also easy to show that

$$\frac{R(q;t)^2}{m}\frac{\partial S\left(q,t\right)}{\partial q} = -\frac{i\ell}{m}\lim_{\delta q \to 0}\frac{\partial Z\left(q,\delta q;t\right)}{\partial\left(\delta q\right)} = \int_{-\infty}^{+\infty}\frac{p}{m}F\left(q,p;t\right)dp\,, \tag{10.12}$$

which gives equation (10.9) its unambiguous interpretation as a continuity equation. The second equation has a derivation with respect to q and thus may be written as

$$\frac{\partial S}{\partial t} + \frac{1}{2m}\left(\frac{\partial S}{\partial q}\right)^2 + V\left(q\right) - \frac{\ell^2}{2mR\left(q;t\right)}\frac{\partial^2 R}{\partial q^2} = f\left(t\right), \tag{10.13}$$

in which the function $f\left(t\right)$ is arbitrary. Since we can redefine $S\left(q;t\right)$ as

$$S^{'}\left(q;t\right) = S\left(q;t\right) + \int_0^t f\left(t'\right)dt'$$

to cancel out the right hand side of the previous equation, we may just consider that $f\left(t\right) = 0$ without loss of generality.

However, equations (10.13) with $f\left(t\right) = 0$ and (10.9) are fully equivalent to the Schrödinger equation

$$-\frac{\hbar^2}{2m}\frac{\partial^2\psi}{\partial q^2} + V\left(q\right)\psi\left(q;t\right) = i\hbar\frac{\partial\psi\left(q;t\right)}{\partial t}\,, \tag{10.14}$$

since, if we replace the definition (10.7) in (10.14) and collect the real and imaginary terms (and make $\ell = \hbar$ to "discover" the value of our universal parameter[1]), we also arrive at the same results (10.9) and (10.13).

This is the complete derivation and it does not depend upon any kind of abstruse mathematics, although the nature of the expansion up to second order must still be clarified. It is well-known that when one assumes that the characteristic function of *any process* should be written up to second order, then the Central Limit Theorem is in place, which is something that can be shown using this approach [8].

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[1] One should remember that no mathematical derivation process can simply "find" the universal parameter of a theory. A similar situation can be found in Gravitation (where G is experimentally obtained) or in Electromagnetism.

10.3 Quantization in Spherical Coordinates: an Example

It is really awful that to quantize a system (to write down its Schrödinger equation) according to some orthogonal curvilinear coordinate system, for instance, one has to first write down its Schrödinger equation in Cartesian coordinates and then change to the desired orthogonal system.

This would imply the embarrassing conclusion that all the formalism depends upon a coordinate system, which is preposterous. There had been trials in the literature to overcome these difficulties [9], but even these approaches are permeated with additional suppositions, where the author has to postulate that the total quantum-mechanical momentum operator p_{q_i} corresponding to the generalized coordinate q_i is given by

$$p_{q_i} = -i\hbar \frac{\partial}{\partial q_i} \tag{10.15}$$

and where one also has to write the kinetic energy term of the classical Hamiltonian as

$$H = \frac{1}{2m} \sum_{ik} p^*_{q_i} g^{ik} p_{q_k} . \tag{10.16}$$

These approaches seem rather unsatisfactory for we would like to derive our results using only first principles, without having to add more postulates to the theory.

On the other hand, if we do have an axiomatic approach, since every formal aspect of the theory should be contained in the axioms (or else they are not a complete set of axioms), the problem of quantization in generalized curvilinear orthogonal coordinate systems *must* also be contained in the axioms in such a way that, having written the axioms in the desired system, one *must* find the Schrödinger equation in this same coordinate system. This is an imposition (and in fact quite a strong one, as we will see) upon the set of axioms. For the sake of clarity and simplicity, we show an example on quantization in spherical coordinates that can be generalized to any coordinate system. We begin rewriting our two axioms in the appropriate coordinate system as:

Axiom 1 *The characteristic function, defined as*

$$Z\left(\vec{r}, \delta\vec{r}; t\right) = \int_{-\infty}^{+\infty} F\left(r, \theta, \phi, p_r, p_\theta, p_\phi; t\right) e^{i\vec{p}\cdot\delta\vec{r}/\hbar} d^3p \, , \tag{10.17}$$

is such that it can be written as

$$Z\left(\vec{r}, \delta\vec{r}; t\right) = \psi^*\left(\vec{r} - \frac{\delta\vec{r}}{2}; t\right) \psi\left(\vec{r} + \frac{\delta\vec{r}}{2}; t\right) , \tag{10.18}$$

and should be expanded up to second order in $\delta\vec{r}$.

Axiom 2 *For an isolated system, the joint phase-space probability density function obeys the integrated Liouville equation*

$$\int \exp\left(i\frac{\vec{p}\cdot\delta\vec{r}}{\hbar}\right) \frac{dF\left(r, \theta, \phi, p_r, p_\theta, p_\phi; t\right)}{dt} = 0 \, . \tag{10.19}$$

From these axioms, all the previous calculations proceed in the same fashion, with the usual complications introduced by the coordinate system. Thus, the classical Hamiltonian in spherical coordinates is given by

$$H = \frac{1}{2m}\left(p_r^2 + \frac{p_\theta^2}{r^2} + \frac{p_\phi^2}{r^2\sin^2\theta}\right) + V\left(\vec{r}\right), \tag{10.20}$$

and the Liouville equation becomes

$$\frac{\partial F}{\partial t} + \frac{p_r}{m}\frac{\partial F}{\partial r} + \frac{p_\theta}{mr^2}\frac{\partial F}{\partial \theta} + \frac{p_\phi}{mr^2\sin^2\theta}\frac{\partial F}{\partial \phi} - \left(\frac{\partial V}{\partial r} - \frac{p_\theta^2}{mr^3} - \frac{p_\phi^2}{mr^3\sin^2\theta}\right)\frac{\partial F}{\partial p_r} + \\ + \frac{p_\phi^2}{mr^2\sin^2\theta}\cot\theta\frac{\partial F}{\partial p_\theta} = 0\,. \tag{10.21}$$

Now, the Fourier transformation in (10.17) can be easily constructed. Note that we have

$$\delta\vec{r} = \delta r\hat{r} + r\delta\theta\widehat{\theta} + r\sin\theta\delta\phi\widehat{\phi}\,, \tag{10.22}$$

where $\left(\hat{r}, \widehat{\theta}, \widehat{\phi}\right)$ are the unit normal vectors, and

$$\vec{p} = p_r\hat{r} + \frac{p_\theta}{r}\widehat{\theta} + \frac{p_\phi}{r\sin\theta}\widehat{\phi}\,, \tag{10.23}$$

giving

$$\vec{p}\cdot\delta\vec{r} = p_r\delta r + p_\theta\delta\theta + p_\phi\delta\phi\,, \tag{10.24}$$

which is a general feature of what is called Mathieu's transformations (see Ref. [10], pp. 201-204), that form a subset of the canonical transformations. Indeed, point transformations are a particular case of Mathieu's transformations.

The relations between the momenta in Cartesian and spherical coordinates are given by

$$\begin{array}{l} p_x = p_r\sin\theta\cos\phi + \frac{p_\theta}{r}\cos\theta\cos\phi - \frac{p_\phi}{r}\frac{\sin\phi}{\sin\theta} \\ p_y = p_r\sin\theta\sin\phi + \frac{p_\theta}{r}\cos\theta\sin\phi + \frac{p_\phi}{r}\frac{\cos\phi}{\sin\theta} \\ p_z = p_r\cos\theta - \frac{p_\theta}{r}\sin\theta \end{array}, \tag{10.25}$$

and the Jacobian relating the two volume elements is given by

$$dp_x dp_y dp_z = \left\|J\right\|_p dp_r dp_\theta dp_\phi\,, \tag{10.26}$$

and thus, since point transformations are canonical and the phase space volume element does not change, we have

$$\left\|J\right\|_p = \frac{1}{r^2\sin\theta}\,. \tag{10.27}$$

With results (10.24) and (10.27) we may write

$$Z\left(\vec{r}, \delta\vec{r}; t\right) = \int F\left(\vec{r}, \vec{p}; t\right) \times \times \exp\left[\frac{i}{\hbar}\left(p_r\delta r + p_\theta\delta\theta + p_\phi\delta\phi\right)\right]\frac{dp_r dp_\theta dp_\phi}{r^2\sin\theta}\,. \tag{10.28}$$

We now impose this transformation upon the Liouville equation (10.21) and use Axiom 1 to find

$$\begin{aligned} &-\frac{\hbar^2}{m}\left[\frac{1}{r^2}\frac{\partial}{\partial r}\left(r^2\frac{\partial Z}{\partial\left(\delta r\right)}\right)+\frac{1}{r^2\sin\theta}\frac{\partial}{\partial\theta}\left(\sin\theta\frac{\partial Z}{\partial\left(\delta\theta\right)}\right)+\frac{1}{r^2\mathrm{sin}^2\theta}\frac{\partial^2 Z}{\partial\phi\partial\left(\delta\phi\right)}\right] \\ &\quad+\frac{\hbar^2}{m}\left[\frac{\delta r}{r^3}\frac{\partial^2 Z}{\partial(\delta\theta)^2}+\frac{\delta r}{r^3\mathrm{sin}^2\theta}\frac{\partial^2 Z}{\partial(\delta\phi)^2}+\frac{\delta\theta\mathrm{cot}\theta}{r^2\mathrm{sin}^2\theta}\frac{\partial^2 Z}{\partial(\delta\phi)^2}\right]+\delta r\frac{\partial V}{\partial r}Z=i\hbar\frac{\partial Z}{\partial t}. \end{aligned} \tag{10.29}$$

To proceed with the calculations we must now write Z in spherical coordinates. We know that it must be written in Cartesian coordinates as

$$\begin{aligned} Z\left(\vec{R},\delta\vec{r};\mathrm{t}\right)=&\left\{R^2+\frac{R}{4}\sum_{i,j=1}^{3}\delta x_i\delta x_J\frac{\partial^2 R}{\partial x_i\partial x_J}-\frac{1}{4}\sum_{i,j=1}^{3}\delta x_i\delta x_J\frac{\partial R}{\partial x_i}\frac{\partial R}{\partial x_J}\right\}\times \\ &\times\exp\left[\frac{i}{\hbar}\left(\delta x\frac{\partial S}{\partial x}+\delta y\frac{\partial S}{\partial y}+\delta z\frac{\partial S}{\partial z}\right)\right], \end{aligned} \tag{10.30}$$

where we used the fact that the $\psi\left(\vec{r};t\right)$ can be written as in (10.7). We now use the fact that

$$\begin{array}{l} \partial_x=\sin\theta\cos\phi\partial_r+\frac{1}{r}\cos\theta\cos\phi\partial_\theta-\frac{1}{r}\frac{\sin\phi}{\sin\theta}\partial_\phi \\ \partial_y=\sin\theta\sin\phi\partial_r+\frac{1}{r}\cos\theta\sin\phi\partial_\theta+\frac{1}{r}\frac{\sin\phi}{\sin\theta}\partial_\phi \\ \partial_y=cos\theta\partial_r-\frac{1}{r}\sin\theta\partial_\theta \end{array}, \tag{10.31}$$

where ∂_u is an abbreviation for $\partial/\partial u$. Thus, in spherical coordinates, the characteristic function becomes (up to second order in δu, $u=r,\theta,\phi$ and their products)

$$\begin{aligned} Z\left(\vec{r},\delta\vec{r};t\right)=&\Big\{R^2+\tfrac{R}{4}\Big[\delta r^2\tfrac{\partial^2 R}{\partial r^2}+\delta\theta^2\left(\tfrac{\partial^2 R}{\partial\theta^2}+r\tfrac{\partial R}{\partial r}\right)\delta\phi^2\left(\tfrac{\partial^2 R}{\partial\phi^2}+r\mathrm{sin}^2\theta\tfrac{\partial R}{\partial r}+cos\theta\sin\theta\tfrac{\partial R}{\partial\theta}\right) \\ &+2\delta r\delta\theta\left(\tfrac{\partial^2 R}{\partial r\partial\theta}-\tfrac{1}{r}\tfrac{\partial R}{\partial\theta}\right)+2r\delta\phi\left(\tfrac{\partial^2 R}{\partial r\partial\phi}-\tfrac{1}{r}\tfrac{\partial R}{\partial\phi}\right)+2\delta\theta\delta\phi\left(\tfrac{\partial^2 R}{\partial\theta\partial\phi}-\mathrm{cot}\theta\tfrac{\partial R}{\partial\phi}\right)\Big] \\ &-\tfrac{1}{4}\left[\delta r^2\left(\tfrac{\partial R}{\partial r}\right)^2+\tfrac{\delta\theta^2}{r^2}\left(\tfrac{\partial R}{\partial\theta}\right)^2+\tfrac{\delta\phi^2}{r^2\mathrm{sin}^2\theta}\left(\tfrac{\partial R}{\partial\phi}\right)^2\right. \\ &\left.+2\tfrac{\delta r\delta\theta}{r}\tfrac{\partial R}{\partial r}\tfrac{\partial R}{\partial\theta}+2\tfrac{\delta r\delta\phi}{r\sin\theta}\tfrac{\partial R}{\partial r}\tfrac{\partial R}{\partial\phi}+2\tfrac{\delta\theta\delta\phi}{r^2\sin\theta}\tfrac{\partial R}{\partial\theta}\tfrac{\partial R}{\partial\phi}\right]\Big\} \\ &\times\exp\left[\tfrac{i}{\hbar}\left(\delta r\tfrac{\partial S}{\partial r}+\delta\theta\tfrac{\partial S}{\partial\theta}+\delta\phi\tfrac{\partial S}{\partial\phi}\right)\right] \end{aligned} \tag{10.32}$$

Substituting this expression into (10.29) and collecting zeroth and first order terms in δr, $\delta\theta$, and $\delta\phi$, we find the following two equations

$$\delta\vec{r}\cdot\frac{\partial}{\partial\vec{r}}\left[\frac{\partial S}{\partial t}+\frac{1}{2m}(\nabla S)^2+V\left(r\right)-\frac{\hbar^2}{2mR}\nabla^2 R\right]=0 \tag{10.33}$$

and

$$\frac{\partial R^2}{\partial t}+\nabla\cdot\left(\frac{R^2}{m}\nabla S\right)=0\,,$$

all written in spherical coordinates (the gradient, the divergent, and the Laplacian differential operators). It is then possible to show that we have the equivalence of these two last equations with the Schrödinger equation given by

$$-\frac{\hbar^2}{2m}\nabla^2\psi\left(\vec{r},t\right)+V\left(r\right)\psi\left(\vec{r},t\right)=i\hbar\frac{\partial\psi\left(\vec{r},t\right)}{\partial t}\,, \tag{10.34}$$

also written in spherical coordinates. To see this, one needs only to write the last equation in spherical coordinates, write

$$\psi = R\left(\vec{r},t\right)\exp\left(\frac{i}{\hbar}S\left(\vec{r},t\right)\right)\ , \tag{10.35}$$

substitute this result in the pervious equation and subtract the overall expression from the one coming from (10.33). This ends our derivation. This procedure, developed for spherical coordinates, can be generalized to any coordinate system.

It is important to note here the non-trivial algebraic relations involved in the derivation. Equation (10.29) is already very complicated and the substitution in it of the extremely complicated expression (10.32) turns the problem into a very long and intricate (although direct) algebraic problem.

It would be an extravagance to believe that the success of the derivation in this case (and all cases related to other coordinate systems) is simply a matter of coincidence. Our confidence in the derivation method and the axioms should increase with the success of this application. When we work out the connection of this derivation (in section 10.5) with Feynman's path integral approach, it is expected that this confidence should also increase.

10.4 Connection to Bohr-Sommerfeld Rules

We have the definition of the characteristic function as given by (10.1) and also the imposition that it must be written as a product of the type shown in (10.2). Since the characteristic function is a Fourier Transformation of the probability density defined upon phase space, if it is a product, then the probability density must be a convolution. We thus write

$$F\left(q,p;t\right) = \int_{-\infty}^{+\infty}\phi^{*}\left(q,2p-p^{'};t\right)\phi\left(q,p^{'};t\right)dp^{'}\ , \tag{10.36}$$

where ϕ is some phase-space probability amplitude. In this case it is easy to show that the integration in (10.1) leads to

$$Z\left(q,\delta q;t\right) = \mathfrak{F}\left\{\phi^{*}\left(q,p;t\right)\right\}\mathfrak{F}\left\{\phi\left(q,p;t\right)\right\}\ ,$$

as desired, so that $\mathfrak{F}\left\{\phi\right\}$ represents the Fourier transformation of ϕ with respect to p.

Now writing (look at the factor two in the denominator)

$$\psi\left(q+\frac{\delta q}{2};t\right) = \mathfrak{F}\left\{\phi\left(q,p;t\right)\right\} = \int\exp\left(\frac{i}{2\hbar}p\delta q\right)\phi\left(q,p;t\right)dp, \tag{10.37}$$

such that

$$\psi^{*}\left(q-\frac{\delta q}{2};t\right) = \mathfrak{F}\left\{\phi^{*}\left(q,p;t\right)\right\} = \int\exp\left(\frac{i}{2\hbar}p\delta q\right)\phi^{*}\left(q,p;t\right)dp, \tag{10.38}$$

we reach the expression in (10.2). Thus, the constraint (10.2) is mathematically equivalent to assume the previous form for $F\left(q,p;t\right)$, and thus, the mathematical form for $\psi\left(q;t\right)$ in terms of $\delta q/2$.

From results (10.37) and (10.38) it is very easy to derive the Bohr-Sommerfeld rules. Consider that we are interested in translating the amplitude $\psi\,(q;t)$ in configuration space from the point q to the point $q+\Delta q$ by infinitesimal transformations δq. In expression (10.37) we can see that the kernel of the infinitesimal transformation is given by

$$K_{p(q)}\,(q+\delta q,q) = \exp\left(\frac{i}{\hbar}p\,(q)\,\delta q\right), \tag{10.39}$$

and we write explicitly the dependence of $p\,(q)$ on variable q to make it clear that we are on a trajectory of the system[2]. The *finite* transformation

$$\psi\,(q;t)\rightarrow\psi\,(q+\Delta q)$$

would imply in the kernel

$$\psi\,(q+\Delta q;t) = \int K_p\,(q+\Delta q,q)\,\phi\,(q,p;t)\,dp\,,$$

such that (the arguments here are quite similar to those of Feynman in his path integral approach[11])

$$K_p\,(q+\Delta q,q) = \lim_{N\rightarrow\infty}\Pi_{n-1}^{N}K_{p(q+(n-1)\delta q)}\,(q+n\delta q,q+(n-1)\,\delta q)\,,$$

where we put $N\delta q=\Delta q$ and take the limit $N\rightarrow\infty$, since Δq is a finite interval and δq is infinitesimal. Using (10.39) we find that this last expression can be written as

$$K_p\,(q+\Delta q,q) = \exp\left(\frac{i}{\hbar}\lim_{N\rightarrow\infty}\sum_{n=0}^{N}p\,(q+n\delta q)\,\delta q\right).$$

The sum in the exponent is clearly an integral taken along the trajectory of the particle and we end up with

$$K_p\,(q+\Delta q,q) = \exp\left(\frac{i}{\hbar}\int_q^{q+\Delta q}p\,(q)\,dq\right).$$

If Δq assesses a *symmetry* of the problem ($q+\Delta q$ can be equal to q for rotations by 2π, for instance) we must impose that

$$\psi\,(q+\Delta q;t) = \pm\psi\,(q;t)\,, \tag{10.40}$$

where the ± sign comes from the fact that $\psi\,(q;t)$ is an amplitude, and the physically important quantity is the density, which allows both signs. Since we can now write

$$\psi\,(q+\Delta q;t) = \int\exp\left(\frac{i}{\hbar}\int_q^{q+\Delta q}p\,(q)\,dq\right)\phi\,(q,p;t)\,dp\,,$$

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[2] If one is distressed by the notion of trajectory, look at Feynman's approach, to be considered in the next section.

we obey (10.40) if we put

$$\exp\left(\frac{i}{\hbar}\int_{q}^{q+\Delta q} p\left(q\right)dq\right)=\pm 1\,.$$

This last expression immediately implies that

$$\int_{q}^{q+\Delta q} p\left(q\right)dq=\begin{cases} 2n\pi\hbar=nh & \text{if } K_p\text{= }+1 \\ 2n\pi\hbar+\pi\hbar=\left(n+\frac{1}{2}\right)h & \text{if } K_p\text{= }-1 \end{cases}\,, \tag{10.41}$$

which is the expression for the Bohr-Sommerfeld rules, with the difference that, from the mathematical derivation, we also find the possibility of half-integral numbers.

This was never predicted in the historical development of the theory and is usually considered as a flaw, since there are a number of situations in which half-integral quantum numbers are necessary (see [12], p. 48). Obviously, this theory can neither assess results related to the probability amplitudes, such as those related to intensities, nor problems without symmetries – except in an approximate way.

However, given the derivation process, relations (10.41) cannot be considered a “mere approximation” for systems showing some kind of symmetry, although it may be assumed as a first approximation (semiclassical is the usual word) for systems in which there is no available symmetry. As with the Feynman approach (that we will present in the next section), the integrals (10.41) give the most or least probable trajectories of the system’s particles, and thus they also furnish the points at which one should expect maxima or minima for the probability density. They may be used to show that it is possible to interpret “ondulatory” phenomena, such as the double slit interferometry, only in terms of particles [13].

10.5 Connections with Feynman’s Path Integral Approach

In this section we are interested in showing that our approach towards the establishment of the Bohr- Sommerfeld conditions is fully equivalent with Feynman’s path integral method [11] (only slight modifications would be necessary). Moreover, in Feynman’s interpretation there appears also a quantity (usually written as ε) representing “infinitesimal amounts of time” ε, which is equivalent to disregarding second order terms in ε.

We begin by writing

$$p\delta q=p\frac{\delta q}{\delta t}\delta t\,,$$

and we put $\dot{q}=\delta q/\delta t$. This means that $\dot{q}$ represents the velocity taken over the same trajectory, since in general we would have

$$\delta q=\Delta q+\dot{q}\delta t\,,$$

where Δq is the separation between two distinct trajectories (which we made equal to zero). We must have

$$\Delta\int_{t_1}^{t_2} p\dot{q}dt=\Delta\int_{q(t_1)}^{q(t_2)} pdq=0\,,$$

which is an expression for the Principle of Least Action. We may now use

$$\dot{q}p = L\left(q, \dot{q}; t\right) - E,$$

where $L\left(q, \dot{q}; t\right)$ is the classical Lagrangian function and E is the energy (supposed constant) of the system under consideration. Our expression (10.37) becomes

$$\psi\left(q\left(t + \frac{\delta t}{2}\right)\right) = \int \exp\left[\frac{i}{2\hbar}\left(L\left(q, \dot{q}; t\right) - E\right)\delta t\right]\phi\left(q, p; t\right) J\left(\frac{p}{\dot{q}}\right) d\dot{q}, \qquad (10.42)$$

where $J\left(p/\dot{q}\right)$ is the Jacobian of the transformation $\left(q, p\right) \to \left(q, \dot{q}\right)$.

The kernel of the infinitesimal (in time) transformation in (10.42) is given by

$$K_{\dot{q}(t)}\left(t + \delta t, t\right) = J\left(\frac{p\left(t\right)}{\dot{q}\left(t\right)}\right)\exp\left[\frac{i}{2\hbar}\left(L\left(q, \dot{q}; t\right) - E\right)\delta t\right],$$

such that the transformation between two different times $t_a = 0$ and $t_b = t$ may be written as

$$K_{\dot{q}(t)}\left(t_b, t_a\right) = \lim_{N \to \infty}\prod_{n=1}^{N} K_{\dot{q}(t+(n-1)\delta t)}\left(t + n\delta t, t + \left(n - 1\right)\delta t\right),$$

where $N\delta t = t_b - t_a$, making it necessary to take the limit $N \to \infty$, since δt is infinitesimal. We may thus write $\left[t_n = t + \left(n - 1\right)\delta t\right]$

$$K_{\dot{q}(t)}\left(t_b, t_a\right) = \left[\lim_{N \to \infty}\prod_{n=1}^{N} J\left(\frac{p\left(t_n\right)}{\dot{q}\left(t_n\right)}\right)\right]\exp\left[\frac{i}{\hbar}\lim_{N \to \infty}\sum\left[L\left(q\left(t_n\right), \dot{q}\left(t_n\right); t\right) - E\right]\delta t\right].$$

In the appropriate limit we get

$$K_{\dot{q}(t)}\left(t_b, t_a\right) = A\exp\left[\frac{i}{\hbar}\int_{t_a}^{t_b}\left[L\left(q\left(t_n\right), \dot{q}\left(t_n\right); t\right)\right]dt - \frac{i}{\hbar}E\left(t_b - t_a\right)\right],$$

where we put

$$A = \lim_{N \to \infty}\prod_{n=1}^{N} J\left(\frac{p\left(t_n\right)}{\dot{q}\left(t_n\right)}\right).$$

Since the classical action is given by

$$S_{cl}\left[t_b, t_a\right] = \int_{t_a}^{t_b} L\left(q, \dot{q}; t\right) dt$$

we finally get the desired result

$$K_{\dot{q}(t)}\left(t_b, t_a\right) = A\exp\left[\frac{i}{\hbar}S_{cl}\left[t_a, t_b\right] - \frac{i}{\hbar}E\left(t_b - t_a\right)\right],$$

which is the expression for the kernel of Feynman's path integral approach. Note that the Feynman approach furnishes the amplitudes and is an alternative approach to the Schrödinger equation. The connection between Feynman's derivation of the Schrödinger equation and ours unravels the deep significance of the expansion up to second order in the parameter δq. This significance is strengthen when we show, in the next section, the connection between these derivations and the Central Limit Theorem.

10.6 Connection to the Central Limit Theorem

It is known that to write a characteristic function up to second order means to assume the Central Limit Theorem. In the present case, the expansion up to second order refers to the variable δq, which is connected to the variable momentum p through the Fourier transform, introduced by the second axiom.

Thus, it is possible to show [8] that, by inversion of the Fourier transform, we get, for the quantum mechanical phase space probability density function, the expression

$$F\left(q,p;t\right)=\frac{\rho\left(q;t\right)}{\left[2\pi\left(-\hbar^{2}\frac{\partial^{2}\ln Z}{\partial(\delta q)^{2}}\right)_{0}\right]^{1/2}}\exp\left\{-\frac{\left[p-\left(-i\hbar\frac{\partial\ln Z}{\partial(\delta q)}\right)_{0}\right]^{2}}{2\left(-\hbar^{2}\frac{\partial^{2}\ln Z}{\partial(\delta q)^{2}}\right)_{0}}\right\}, \qquad (10.43)$$

With this result at hand, we can understand the implications of having the Liouville equation integrated, as presented in axiom 2.

Another point that needs clarification is the fact that the probability distribution function $F\left(q,p;t\right)$, when substituted back in the Liouville equation *does not satisfy it* for each phase space point (q,p). In fact, this function satisfies only the momentum integrated version of the Liouville equation, for which we have

$$\int p^{k}L_{op}\left(F\left(q,p;t\right)\right)dp=0,\ k=0,1,2$$

where L_{op} is the Liouville operator.

In fact, if we substitute $F\left(x,p;t\right)$ into the (non-integrated) Liouville equation, we end, after some straightforward calculations, with the expression[3]

$$\frac{L_{op}\left\{F\left(q,p;t\right)\right\}}{F(q,p;t)}=\rho\frac{\partial v}{\partial q}\left\{p[p-p(q,t)]^{2}-2v\left[p-p(q,t)\right]-vp\right\}+ \\ +m\rho\frac{\partial v}{\partial t}\left\{[p-p(q,t)]^{2}-v\right\}+2\frac{\partial p(q,t)}{\partial q}\rho v\left\{[p-p(q,t)]^{2}-v\right\}.$$

Now, it can be shown that the term $\partial v/\partial t$ can be put in the form

$$m\frac{\partial v}{\partial t}=-\frac{\partial v}{\partial q}p\left(q,t\right)-2v\frac{\partial p(q,t)}{\partial q}+\frac{\hbar^{2}}{4}\frac{\partial^{3}p(q,t)}{\partial q^{3}}+\frac{\hbar^{2}}{4\rho}\frac{\partial^{2}p(q,t)}{\partial q^{2}}\frac{\partial\rho}{\partial q}.$$

and substitution of this term in the previous equation gives, for the most usual case in which we have $\partial^{2}p(x,t)/\partial x^{2}$ and $\partial^{3}p(x,t)/\partial x^{3}$ both equal to zero and thus

$$L_{op}\left\{F\left(q,p;t\right)\right\}=\frac{1}{2m}\frac{\partial v}{\partial q}\left\{\frac{[p-p(q,t)]^{2}}{v(q,t)}-3\right\}.$$

Thus, if we substitute the probability density function (10.43) into the Liouville equation, we do not have an exact analytic solution. But how close to a solution we get? To see the

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[3] We divided by $F(q,p;t)$ to eliminate the asymptotic exponential decay of this function.

answer to that question for a specific problem one can consider the harmonic oscillator problem and calculate the following quantity

$$s_n\left(q,p;t\right)=\frac{L_{op}\left\{F_n\left(q,p;t\right)\right\}}{F_n\left(q,p;t\right)}.$$

For the states $n = 1, 2$ of the harmonic oscillator we have the results shown in Figure 10.1, where it is obvious that the function $s_n\left(q, p; t\right)$ becomes different from zero (F_n is not a solution of the Liouville operator) only at the points where we can find high values of the fluctuations.

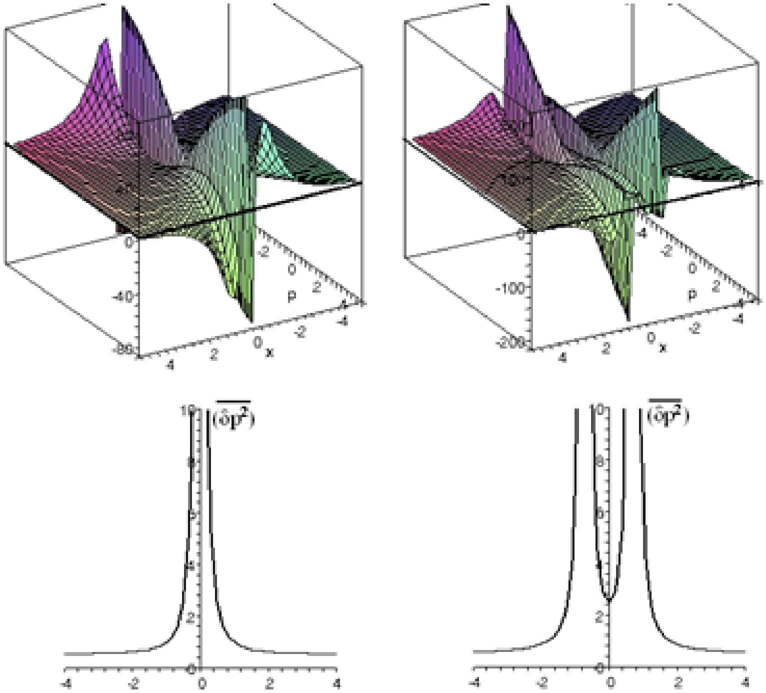

Figure 10.1: Fluctuation profiles of s_n for $n = 1, 2$ of the harmonic oscillator. The functions are solutions of the Liouville equation, except in the vicinity of the points at which fluctuations are maxima. Each fluctuation pattern is shown in the images above. The integration in axiom 2 makes these fluctuations compensate and give zero.

This means that we are very close to a solution, but we failed to take into account the detailed aspect of the fluctuations when we used the Liouville equation—as it is obvious from the fact that this equation does not take into account such a behavior.

At this point, we assume that the reader is rather convinced of the mathematical adequacy of our quantization method. Thus, we pass on to extend it to embrace dissipation.

10.7 Introducing dissipation

We know that, for Hamiltonian systems, the phase space volume behaves as an incompressible fluid. However, when dissipative forces are present, this volume can shrink or expand in a way that we will show in what follows.

We consider an infinitesimal phase space volume element $\delta\vec{x}\delta\vec{p}$. The term δN gives the number of systems in this volume at time t with coordinates in the interval $[\vec{x},\vec{x}+\delta\vec{x}]\times[\vec{p},\vec{p}+\delta\vec{p}]$ and is given by

$$\delta N = F(\vec{x},\vec{p},t)\delta\vec{x}\delta\vec{p},$$

where F is the phase space probability density function. This function must be such that

$$\int F(\vec{x},\vec{p},t)d\vec{x}d\vec{p} = N\,,$$

since the overall number of systems will be kept fixed.

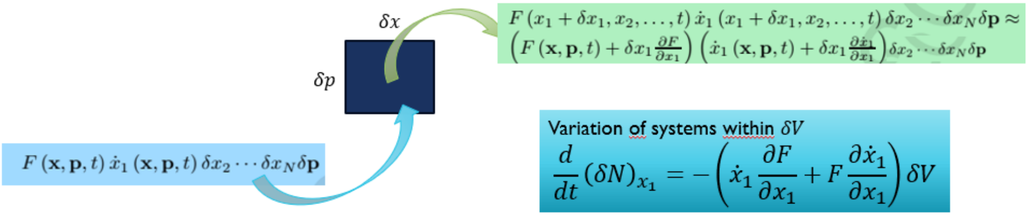

Figure 10.2: The process of dissipation within a phase space cell.

Now, since we have dissipation, we may assume that, at some instant of time, the number of systems entering the phase space cell $[\vec{x}+\delta\vec{x},\vec{p}+\delta\vec{p}]$ through some face will be different from the number of systems leaving this same phase space cell through an opposite face. For the faces normal to x_1 axis located at x_1 and $x_1+\delta x_1$ the fraction of systems entering into the phase space cell is given by (see Figure 10.2)

$$F(\vec{x},\vec{p},t)\dot{x}_1(\vec{x},\vec{p},t)\delta x_2\cdots\delta x_N\delta\vec{p},$$

while the fraction of systems leaving this phase space cell is just

$$F(x_1+\delta x_1,x_2,\ldots,x_N,\vec{p},t)\dot{x}_1(x_1+\delta x_1,x_2,\ldots,x_N,\vec{p},t)\delta x_2\cdots\delta x_N\delta\vec{p}\approx$$
$$\approx\left(F(\vec{x},\vec{p},t)+\delta x_1\frac{\partial F}{\partial x_1}\right)\left(\dot{x}_1(\vec{x},\vec{p},t)+\delta x_1\frac{\partial \dot{x}_1}{\partial x_1}\right)$$

and, thus,

$$\frac{d}{dt}(\delta N)_{x_1} = -\left(\dot{x}_1\frac{\partial F}{\partial x_1}+F\frac{\partial \dot{x}_1}{\partial x_1}\right)\delta\vec{x}\delta\vec{p}.$$

If we now sum all the contributions from all directions and also from the momenta we get the total time variation of the number of systems within the phase space cell element as [7]

$$\frac{d(\delta N)}{dt} = -\left[\left(\nabla_{\vec{x}}\cdot\dot{\vec{x}}+\nabla_{\vec{p}}\cdot\dot{\vec{p}}\right)F+\dot{\vec{x}}\cdot\frac{\partial F}{\partial\vec{x}}+\dot{\vec{p}}\cdot\frac{\partial F}{\partial\vec{p}}\right]\delta\vec{x}\delta\vec{p}, \qquad (10.44)$$

which may be written also as

$$\frac{d(\delta N)}{dt} = -\left(\nabla_{\vec{x}} \cdot (\dot{\vec{x}}F) + \nabla_{\vec{p}} \cdot (\dot{\vec{p}}F)\right) \delta\vec{x}\delta\vec{p},$$

which is a divergence within a phase space cell. Now, since

$$\frac{1}{\delta\vec{x}\delta\vec{p}}\frac{d(\delta N)}{dt} = \frac{\partial f}{\partial t},$$

we get

$$\frac{dF}{dt} = -\Lambda(\vec{x},\vec{p},t)F(\vec{x},\vec{p},t), \tag{10.45}$$

where $\Lambda(\vec{x},\vec{p},t)$ is called the *compression factor* and is given as

$$\Lambda(\vec{x},\vec{p},t) = \nabla_{\vec{x}} \cdot (\dot{\vec{x}}) + \nabla_{\vec{p}} \cdot (\dot{\vec{p}}).$$

Note that if the system is Hamiltonian, we have $\dot{\vec{x}} = \nabla_{\vec{p}} H$ and $\dot{\vec{p}} = -\nabla_{\vec{x}} H$, we get the usual Liouville equation .

10.7.1 Quantization

We now use the previous equation (10.45) to make our quantization in exactly the same way we have already done (see [7] for details). If we assume the equation

$$\frac{\vec{p}}{dt} = -\nabla V(\vec{x}) - \frac{\gamma}{m}\vec{p}, \tag{10.46}$$

and keep the axioms as they were presented for the Hamiltonian case, we get, after some straightforward calculations, the result

$$\delta\vec{x} \cdot \nabla\left[\frac{\partial S}{\partial t} = -\left(\frac{(\nabla S)^2}{2m} + V(\vec{x}) - \frac{\hbar^2}{2mR}\nabla^2 R\right) - \frac{\gamma}{m}S\right], \tag{10.47}$$

which is Bohm's equation with the extra term on the right, that is

$$\frac{\partial\vec{p}(\vec{x},t)}{\partial t} = -\nabla_{\vec{x}} H_B(\vec{x},t) - \frac{\gamma}{m}\vec{p}(\vec{x},t),$$

which is just equation (10.46) in terms of the Bohmian formalism. The last term on the right can be written as

$$S = -\frac{i\hbar}{2} \cdot \ln\left(\frac{\psi(\vec{x},t)}{\psi^*(\vec{x},t)}\right),$$

which takes the usual Schrödinger equation into a non-linear Schrödinger equation[7]. This makes the equation too difficult to solve. It would be better if we find a linear equation. We thus change our first axiom to write the characteristic function as

$$\zeta(\vec{x},\vec{p},t) = \int F(\vec{x},\vec{p},t)\exp\left(\frac{i\vec{p}\cdot\delta\vec{x}}{\hbar e^{-\frac{\gamma t}{m}}}\right)d\vec{p} = \psi^*\left(\vec{x} - \frac{\delta\vec{x}}{2}, t\right)\psi\left(\vec{x} + \frac{\delta\vec{x}}{2}\right). \tag{10.48}$$

It is possible to show (see [7]) that this eliminates the rightmost term in the previous equations and we end up with the equation (for ζ, the new characteristic function) as

$$-\frac{\hbar^2 e^{-\frac{2\gamma t}{m}}}{m}\frac{\partial^2\zeta}{\partial\vec{x}\cdot\partial\delta\vec{x}}+\frac{\partial V}{\partial\vec{x}}\cdot\delta\vec{x}\zeta=i\hbar e^{-\frac{\gamma t}{m}}\frac{\partial\zeta}{\partial t}\,. \tag{10.49}$$

We may now repeat all the steps of section 10.2 to get the generalized Schrödinger equation

$$-\frac{\hbar^2 e^{-\frac{2\gamma t}{m}}}{2m}\nabla^2\psi(\vec{x},t)+V(x)\psi(\vec{x},t)=i\hbar e^{-\frac{\gamma t}{m}}\frac{\partial\psi(\vec{x},t)}{\partial t}\,, \tag{10.50}$$

which is the equation we was searching for (note that it is a *linear equation* and, of course, it gives the usual Schrödinger equation if $\gamma=0$). With these changes, the Heisenberg inequality becomes

$$\Delta x_i\Delta p_i\geq\frac{\hbar}{2}e^{-\frac{\gamma t}{m}}\,, \tag{10.51}$$

which clearly states the fact that the momentum (the movement) must decay with the action of a dissipation force. Now we may ask ourselves what effect would this have in the solutions of the equation, that is, in the behavior of quantum mechanical *states*.

Our next step, thus, is to try to solve this equation for a free wave-packet acted by a phenomenological dissipation force. We do that in the next section.

10.8 The "Free" wave packet as an example

The equation is

$$-\frac{\hbar^2 e^{-2\omega t}}{2m}\frac{\partial^2\psi}{\partial x^2}=i\hbar e^{-\omega t}\frac{\partial\psi}{\partial t} \tag{10.52}$$

which means that (with the correct initial conditions)

$$\psi\left(x,t\right)=\exp\left[i\left(K\left(x-x_0\right)-\frac{K^2\hbar}{2m\omega}(1-e^{-\omega t})\right)\right] \tag{10.53}$$

where, for very small values of t,

$$\psi\left(x,t\right)=\exp\left[i\left(K\left(x-x_0\right)-\frac{K^2\hbar}{2m\omega}(1-e^{-\omega t})\right)\right]\simeq e^{i\left(K(x-x_0)-\frac{K^2\hbar}{2m}t\right)}, \tag{10.54}$$

the wave-function without dissipation (since dissipation had not time to work yet). In fact, this result helps us to correctly define the initial conditions – for very small time, we have a free particle with momentum $\hbar K$ and energy $\hbar^2K^2/2m$.

To construct the wave-packet[4], write the structure factor as

$$A\left(k\right)=\frac{b}{\sqrt{2\pi}}e^{-\frac{b^2}{2}(K-K_0)^2}\,, \tag{10.55}$$

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[4] Note that the equation is *linear* and thus we may construct the wave-packet as the superposition of "free" particle solutions.

where b is a constant defining the inverse of the variance of the Gaussian shaped structure factor. We may now construct the Gaussian wave-packet as

$$\begin{aligned}\psi_G\left(x,t\right) &= \tfrac{b}{\sqrt{2\pi}}\int_{-\infty}^{+\infty} e^{-\frac{b^2}{2}(K-K_0)^2} e^{i\left(K(x-x_0)-\frac{K^2\hbar}{2m\omega}\left(1-e^{-\omega t}\right)\right)}dK = \\ &= \tfrac{b}{\sqrt{2\pi}}e^{-\frac{b^2K_0^2}{2}}\int_{-\infty}^{+\infty} e^{-\left(\frac{b^2}{2}+\frac{i\hbar}{2m\omega}\left(1-e^{-\omega t}\right)\right)K^2} e^{\left(b^2K_0+i(x-x_0)\right)K}dK\end{aligned}$$

which gives

$$\psi_G\left(x,t\right) = \frac{b}{\sqrt{2\pi}}e^{-\frac{b^2K_0^2}{2}}\int_{-\infty}^{+\infty} e^{-\beta^2K^2}e^{\alpha K}dK$$

if we put

$$\begin{gathered}\beta^2 = \tfrac{b^2}{2}+\tfrac{ih}{2m\omega}\left(1-e^{-\omega t}\right) \\ \alpha = b^2K_0 + i\left(x-x_0\right)\end{gathered}$$

Now

$$\begin{aligned}\psi_G\left(x,t\right) &= \tfrac{b}{\sqrt{2\pi}}e^{-\frac{b^2K_0^2}{2}}e^{\frac{\alpha^2}{4\beta^2}}\int_{-\infty}^{+\infty} e^{-\left(\beta K-\frac{\alpha}{2\beta}\right)^2}dK = \\ &= \tfrac{b}{\beta\sqrt{2}}e^{-\frac{b^2K_0^2}{2}}e^{\frac{\alpha^2}{4\beta^2}}\end{aligned} \tag{10.56}$$

where α and β^2 are complex numbers and β^2 has a positive real part, which is $b^2/2$. We want to construct the probability density function. Thus, we write

$$\rho_G\left(x,t\right) = \frac{b^2}{2\beta\beta^*}e^{-b^2K_0^2}e^{\frac{\alpha^2}{4\beta^2}}e^{\frac{\alpha^{*2}}{4\beta^{*2}}}\ .$$

Since

$$\beta^2\beta^{*2} = \left(\frac{b^2}{2}+\frac{i\hbar}{2m\omega}\left(1-e^{-\omega t}\right)\right)\left(\frac{b^2}{2}-\frac{i\hbar}{2m\omega}\left(1-e^{-\omega t}\right)\right)\ ,$$

we get

$$\beta^2\beta^{*2} = \frac{1}{4}b^4\left(1+\frac{\hbar^2\left(1-e^{-\omega t}\right)^2}{m^2\omega^2b^4}\right)\ ,$$

and thus

$$\beta\beta^* = \frac{b^2}{2}\left(1+\frac{h^2\left(1-e^{-\omega t}\right)^2}{m^2\omega^2b^4}\right)^{1/2}\ .$$

We now must calculate

$$\begin{aligned}\tfrac{\alpha^2\beta^{*2}+\alpha^{*2}\beta^2}{4\beta^{*2}\beta^2} &= \tfrac{\left(b^2K_0+i(x-x_0)\right)^2\left(\frac{b^2}{2}-\frac{ih}{2m\omega}\left(1-e^{-\omega t}\right)\right)+\left(b^2K_0-i(x-x_0)\right)^2\left(\frac{b^2}{2}+\frac{ih}{2m\omega}\left(1-e^{-\omega t}\right)\right)}{4\beta^{*2}\beta^2} \\ &= \tfrac{-b^2(x-x_0)^2+b^6K_0^2+2b^2K_0(x-x_0)\hbar\left(\frac{1-e^{-\omega t}}{m\omega}\right)}{b^4\left(1+\frac{\hbar^2\left(1-e^{-\omega t}\right)^2}{m^2\omega^2b^4}\right)}\end{aligned}\ ,$$

so that the probability density function becomes

$$\begin{aligned}\rho_G\left(x,t\right) \quad &= \quad \frac{1}{\left(1+\frac{\hbar^2\left(1-e^{-\omega t}\right)^2}{m^2\omega^2b^4}\right)^{1/2}}e^{-b^2K_0^2} \\ &\quad\times\exp\left(\frac{-b^2\left(x-x_0\right)^2+b^6K_0^2+2b^2K_0\left(x-x_0\right)\hbar\left(\frac{1-e^{-\omega t}}{m\omega}\right)}{b^4\left(1+\frac{h^2\left(1-e^{-\omega t}\right)^2}{m^2\omega^2b^4}\right)}\right)\ .\end{aligned}$$

If we complete squares, we get

$$\rho_G\left(x,t\right)=\frac{1}{\left(1+\frac{\hbar^2(1-e^{-\omega t})^2}{m^2\omega^2b^4}\right)^{1/2}}\exp\left(-\frac{\left(\left(x-x_0\right)-\frac{\hbar K_0}{m\omega}\left(1-e^{-\omega t}\right)\right)^2}{b^2\left(1+\frac{\hbar^2(1-e^{\omega t})^2}{m^2\omega^2b^4}\right)}\right). \tag{10.57}$$

This last result shows that our wave-packet has a Gaussian format, that it begins its movement with its peak at the position x_0 and moves with average momentum initially given by $\hbar K_0$. Furthermore, it has a right mean square given by

$$\sigma^2=\frac{b^2}{2}\left(1+\frac{\hbar^2(1-e^{-\omega t})^2}{m^2\omega^2b^4}\right). \tag{10.58}$$

This means that the wave-packet begins with a variance of $b^2/2$ and ends (asymptotically) with the value given by

$$\sigma^2_{t\to\infty}=\frac{b^2}{2}\left(1+\frac{\hbar^2}{m^2\omega^2b^4}\right), \tag{10.59}$$

which shows that the variance of the wave-packet grows up to an asymptotic value, while the wave-packet, asymptotically, becomes

$$\rho_G\left(x\right)=\frac{1}{\left(1+\frac{\hbar^2}{m^2\omega^2b^4}\right)^{1/2}}\exp\left(-\frac{\left(\left(x-x_0\right)-\frac{\hbar K_0}{m\omega}\right)^2}{b^2\left(1+\frac{\hbar^2}{m^2\omega^2b^4}\right)}\right). \tag{10.60}$$

This wave-packet is not time dependent anymore, meaning that it has stopped at the position

$$x_{t\to\infty}=x_0+\frac{\hbar K_0}{m\omega}. \tag{10.61}$$

In this sense, $\omega=T_c^{-1}$ represents the inverse of the characteristic time that the wave-packet takes to stop, since the previous equation can be written as

$$x_{t\to\infty}=x_0+v_0T_c, \tag{10.62}$$

where we put the initial average velocity $v_0=\hbar K_0/m$.

10.9 Conclusions

Quantization, that is, the passage from classical mechanics to quantum mechanics represented by the Schrödinger equation, should be considered an essential element of any quantum mechanical approach. Indeed, as we have shown, the quantization method is capable of inducing a variety of important results regarding the underlying theory. Some of these results were shown in the previous sections.

Moreover, having such a method at hand, one can envisage *extensions* of this method to encompass other physical situations not initially at sight (thus, it is possible, for instance, to easily extend the theory to take into account relativistic effects[14]).

An important extension of the usual Hamiltonian approach is to find ways to derive a Schrödinger-like formalism that encompass dissipation in the way it is commonly treated in classical mechanics, that is, in phenomenological terms, by assuming a dissipation force of the type $-kv$, where k is the phenomenological constant (into which we put a number of details of the system leading to dissipation, as usual). Such an equation was found in a previous work and derived again in this text to show how it is a quite natural extension of the quantization method. The result, thus, was a Generalized Schrödinger equation.

In classical mechanics, one expects that the dissipation force $-kv$ will, after some time, make the movement of the system to stop. One should, thus, ask if such a behavior would be expected on the quantum-mechanical "side". To answer this question, we have considered the movement of the quantum mechanical free wave-packet subjected to the dissipation force $-kv$. As we have shown, the overall quantum mechanical behavior is exactly the same as it is in the classical domain: after some characteristic time T_c, the wave-packet stops its movement (and also stops the diffusion process by which its Gaussian mean square displacement grows without limit). In other words, the wave-packet just stops, as expected. This should be evident from the Generalized Heisenberg relation, showing that the phase space volume shrinks as time goes by.

Such a result may be relevant in some applications of quantum mechanics (mainly in those that are taken with respect to mesoscopic physical situations, where dissipation can be expected). A possible line of application, for instance, could be enhancing the trapping of quantum mechanical systems within some small space (e.g. as with quantum dots), since dissipation can be used to "freeze" the physical system under scrutiny. This can be used to eliminate (or strongly decrease) the amount of loss of trapped physical systems by means of tunnel effects (by freezing them "far" from the walls of the container).

Finally, it is important to note that this quantization approach differs from the usual method to plug a complex potential into the Schrödinger equation – such an approach would mean the appearance of metastable states, instead of the "freezing" above mentioned, and change the unitary behavior of the quantum mechanical system[5]. In fact, this usual approach *can* be also derived from the postulates presented in this work by adding a simple extension of them, but such a development would take us too far afield and thus we leave it for a future development.

10.10 References

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[5] The Generalized Schrödinger equation derived in this work *still represents a unitary behavior*, although one of a more complicated time structure.

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