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Ordering ambiguity versus representation

A de Souza Dutra

Abdus Salam ICTP, Strada Costiera 11, 34014 Trieste, Italy
and
UNESP-Campus de Guaratinguetá-DFQ[1], Av. Dr. Ariberto Pereira da Cunha, 333, C.P. 205, 12516-410 Guaratinguetá SP, Brazil

E-mail: dutra@feg.unesp.br

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Abstract
In this work we show that the ordering ambiguity on quantization depends on the representation choice. This property is then used to solve unambiguously some particular systems. Finally, we speculate on the consequences for more involved cases.

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The problem of ordering ambiguity is one of the long-standing questions of quantum mechanics. This question has attracted the attention of some of the founders of quantum mechanics. Born and Jordan, Weyl, Dirac and von Newmann worked on this matter, as can be verified from the excellent review by Shewell [1]. This is a difficult problem which has advanced very little during the past few decades. Notwithstanding, as a consequence of its importance in some experimental situations, such as impurities in crystals [2–4], the dependence of nuclear forces on the relative velocity of two nucleons [5, 6], and more recently the study of semiconductor heterostructures [7, 8], the interest in such kind of systems never vanished. Furthermore, taking into account the spatial variation of the semiconductor type, some effective Hamiltonians were proposed with a spatially dependent mass for the carrier [9–14]. Finally, recently this matter appeared in some ordering problems [15] and equations with spatially dependent masses [16], both related to D-branes in quantum field theories. Some time ago we discussed the exact solvability of some classes of Hamiltonians with ordering ambiguity [17]. In fact, the problem of the spatially dependent mass has been a growing interest over the past few years [17–34].

Here we observe that there exists a different ordering dependence in different representations, particularly we exploit this feature, by noting that in each one of the more usual representations, the coordinate and the momentum one, there exist a family of classical functions like $f(x)g(p)$, whose quantization is unambiguous. Explicitly, the quantization of $(ax + b)g(p)$ is unambiguous in the momentum representation, and $(cp + d)f(x)$ is

[1] Permanent institution.

unambiguous in the coordinate representation, where a, b, c, d are arbitrary constants. In general, however, the function $f(x)g(p)$ is ambiguous in both representations.

Let us now present the idea we are interested to develop in this work by illustrating it through the study of a concrete example. For this, we remember that in [17] it was shown that for a system whose quantum Hamiltonian has as one of its parts an operator version of the classical function $f(x)p$ the quantization is unambiguous in the coordinate representation. In that representation its Hermitian operator counterpart can be written as

$$f(x)p \to \frac{f^{\alpha}(\hat{x})\hat{p}f^{\beta}(\hat{x}) + f^{\beta}(\hat{x})\hat{p}f^{\alpha}(\hat{x})}{2}, \tag{1}$$

where $\alpha + \beta \equiv 1$. By using the usual coordinate representation for the operator $\hat{p}$, and manipulating the above operator in order to put it to the right, one can see that one obtains for instance

$$f^{\alpha}(\hat{x})\hat{p}f^{\beta}(\hat{x}) = f(\hat{x})\hat{p} - \mathrm{i}\hbar\beta\frac{\mathrm{d}f(\hat{x})}{\mathrm{d}\hat{x}}. \tag{2}$$

Now, using the corresponding operator for $f^{\beta}(\hat{x})\hat{p}f^{\alpha}(\hat{x})$, and then calculating the Hermitian operator (1) with these features, one gets finally

$$\frac{f^{\alpha}(\hat{x})\hat{p}f^{\beta}(\hat{x}) + f^{\beta}(\hat{x})\hat{p}f^{\alpha}(\hat{x})}{2} = f(\hat{x})\hat{p} - \frac{\mathrm{i}\hbar}{2}\frac{\mathrm{d}f(\hat{x})}{\mathrm{d}\hat{x}}, \tag{3}$$

from which we conclude that there is no ordering ambiguity in this representation and any ordering used will conduce essentially to the same final answer, as observed in [17, 18]. However, despite being an important case of ordering, due to its application to the case of the minimal gauge coupling, it cannot be used by itself as a Hamiltonian, at least as a usual non-relativistic one, because the momentum appears linearly in it. Note, however, that in the relativistic case of the Dirac equation [19], the momentum appears linearly and one can think the spatial dependence as a consequence of the spacetime curvature [20].

At this point we introduce the main idea underlying this work, remembering that one could interchange the role of x and p, and discussing the case of the quantization of the classical function $g(p)x$ in the momentum representation. It is not hard to conclude, through an absolutely analogous analysis in the momentum representation, that the Hermitian quantization of this function is unambiguous, and looks like

$$\frac{g^{\alpha}(\hat{p})\hat{x}g^{\beta}(\hat{p}) + g^{\beta}(\hat{p})\hat{x}g^{\alpha}(\hat{p})}{2} = g(\hat{p})\hat{x} + \frac{\mathrm{i}\hbar}{2}\frac{\mathrm{d}g(\hat{p})}{\mathrm{d}\hat{p}}. \tag{4}$$

Note, however, that this operator is surely ambiguous in the coordinate representation. From the above calculation we can conclude that the ordering ambiguity has a dependence on the choice of representation and, as far we know, this feature was not taken into account in the literature up to now. Furthermore, this last operator can be thought of as a Hamiltonian if we choose $g(\hat{p}) = \hat{p}^2$. In this special case, we would have a system with a mass dependence in the spatial coordinate $\left(m(x) \sim \frac{1}{x}\right)$. This is an example of a Hamiltonian which is ambiguous in the coordinate representation and not in the momentum one. In cases like this, one could calculate the wave function in the momentum representation and then transform it through

$$\psi(x,t) = \frac{1}{\sqrt{2\pi\hbar}}\int \mathrm{d}p\tilde{\psi}(p,t)\,\mathrm{e}^{\frac{\mathrm{i}}{\hbar}px} \tag{5}$$

to the coordinate representation if necessary.

For the sake of concreteness, from now on we discuss this case with more details. Firstly, the time-independent wave function equation in the momentum representation is given by

$$\mathrm{i}\hbar p^2\frac{\mathrm{d}\tilde{\psi}(p)}{\mathrm{d}p} + \mathrm{i}\hbar p\tilde{\psi}(p) = E\tilde{\psi}(p). \tag{6}$$

After a straightforward calculation, one obtains for the unambiguous wave function in the momentum representation

$$\tilde{\psi}(p) = N\frac{e^{(\frac{i}{\hbar}\frac{E}{p})}}{p}, \tag{7}$$

where N is an arbitrary integration constant. We can now calculate its Fourier transform, in order to obtain the corresponding coordinate representation wave function. So, we must perform the following integration

$$\psi(x) = \frac{N}{\sqrt{2\pi\hbar}}\int_{-\infty}^{\infty}\frac{dp}{p}\, e^{[\frac{i}{\hbar}(\frac{E}{p}+px)]}. \tag{8}$$

In order to reach this goal, we separate the integral in two sectors, that for the positive p and that for the negative ones. So we get

$$\psi(x) = \frac{N}{\sqrt{2\pi\hbar}}\left\{\int_{\infty}^{0}\frac{dp}{p}\, e^{-[\frac{i}{\hbar}(\frac{E}{p}+px)]} + \int_{0}^{\infty}\frac{dp}{p}\, e^{[\frac{i}{\hbar}(\frac{E}{p}+px)]}\right\}, \tag{9}$$

which after some manipulations can be rewritten as

$$\psi(x) = \frac{2iN}{\sqrt{2\pi\hbar}}\int_{0}^{\infty}\frac{dp}{p}\sin\left[\frac{i}{\hbar}\left(\frac{E}{p}+px\right)\right]. \tag{10}$$

Then, after using the usual trigonometric identities and the known result

$$\int_0^\infty \frac{du}{u}\sin(au)\cos\left(\frac{b}{u}\right) = \frac{\pi}{2}J_0\big(2(a^2b^2)^{\frac{1}{4}}\big) = \int_0^\infty \frac{du}{u}\sin\left(\frac{b}{u}\right)\cos(au), \tag{11}$$

where $J_0(z)$ is the Bessel function of the first kind. One obtains finally that

$$\psi(x) = \sqrt{\frac{2\pi}{\hbar}}\, iN J_0\left(\frac{2}{\hbar}\sqrt{|Ex|}\right). \tag{12}$$

Had we started in the coordinate representation, the wave function equation to be solved would have been

$$x^2\frac{d^2\psi(x)}{dx^2} + x\frac{d\psi(x)}{dx} - \alpha\gamma\psi(x) = -\left(\frac{E}{\hbar^2}\right)x\psi(x), \tag{13}$$

where we ordered the operator coming from xp^2 using

$$O_p \equiv \tfrac{1}{2}(\hat{x}^\alpha\hat{p}\hat{x}^\beta\hat{p}\hat{x}^\gamma + \hat{x}^\gamma\hat{p}\hat{x}^\beta\hat{p}\hat{x}^\alpha) = \hat{x}\hat{p}^2 - i\hbar\hat{p} + \alpha\gamma\hat{x}^{-1}, \tag{14}$$

and we used that $\alpha+\beta+\gamma = 1$. It can be noted that if we make the variable transformation $|x| = \frac{\hbar^2}{4E}w$, the above equation can be cast in the form

$$w^2\frac{d^2\psi}{dw^2} + w\frac{d\psi}{dw} + (w^2 - 4\alpha\gamma)\psi = 0, \tag{15}$$

which is the differential equation of the first kind Bessel function. So, we get finally that in the coordinate representation the ambiguous wave function is expressed as

$$\psi(x) = \tilde{N}J_{\alpha\gamma}\left(\frac{2}{\hbar}\sqrt{|Ex|}\right), \tag{16}$$

once E is positive definite. We conclude that the compatibility of the solutions coming from the two representations requires us to fix one of the parameters appearing in the index of the Bessel function ($\alpha = 0$ or $\gamma = 0$) in the coordinate representation. At this point we should say that one could work with a little bit more general model, where $2m(x) = (ax+b)^{-1}$.

It is not difficult to verify, after straightforward and analogous calculations, that one ends correspondingly in this situation to

$$\psi(x) = \tilde{N} J_0 \left(\frac{2}{\hbar} \sqrt{\left| E \left(x + \frac{b}{a} \right) \right|} \right). \tag{17}$$

As a consequence of the symmetry between these parameters in the operator definition, it is equivalent to choose any of them equal to zero. Choosing to make $\gamma = 0$, we conclude that $\beta = 1 - \alpha$, and we end with a subclass of operators, compatibles in both representations,

$$O_\alpha = \tfrac{1}{2}(\hat{x}^\alpha \hat{p} \hat{x}^{1-\alpha} \hat{p} + \hat{p} \hat{x}^{1-\alpha} \hat{p} \hat{x}^\alpha). \tag{18}$$

Note that the case of the Li and Khun ordering [13], which it was shown to be equivalent to the Weyl ordering [17, 18], corresponds to the choice $\alpha = \frac{1}{2}$.

Below we are going to prove that, in fact, there is no remaining ambiguity because all choices of α are equivalent. For this we note that

$$\begin{aligned} \hat{x}^\alpha \hat{p} \hat{x}^{1-\alpha} \hat{p} &= \sqrt{\hat{x}} \hat{p} \sqrt{\hat{x}} \hat{p} + \mathrm{i}\hbar \left(\alpha - \frac{1}{2} \right) \hat{p}, \\ \hat{p} \hat{x}^{1-\alpha} \hat{p} \hat{x}^\alpha &= \hat{p} \sqrt{\hat{x}} \hat{p} \sqrt{\hat{x}} - \mathrm{i}\hbar \left(\alpha - \frac{1}{2} \right) \hat{p}, \end{aligned} \tag{19}$$

so that the operator O_α is simply rewritten as

$$O_\alpha = \tfrac{1}{2}(\sqrt{\hat{x}} \hat{p} \sqrt{\hat{x}} \hat{p} + \hat{p} \sqrt{\hat{x}} \hat{p} \sqrt{\hat{x}}) = O_{\mathrm{Weyl}}. \tag{20}$$

So we have finally demonstrated that, at least for this particular case, we have been able to avoid the ordering ambiguity by working in the momentum representation. In fact, this conclusion is still true if we include a binding potential energy in the original Hamiltonian. Furthermore, we have shown that this unambiguous quantization corresponds to the so-called Weyl ordering. One can show also that, for a given class of potentials, the problem can be even exactly solvable. Let us illustrate this argument through the study of a particular example, where the calculations can be done analytically up to the very end. The classical Hamiltonian to be considered next is

$$H = (ax + b) p^2 + V(x), \tag{21}$$

which in the coordinate representation (using $\alpha = 0$ or $\gamma = 0$) renders the time-independent equation

$$-\hbar^2 (ax + b) \frac{\mathrm{d}^2 \psi}{\mathrm{d}x^2} - \hbar^2 \frac{\mathrm{d}\psi}{\mathrm{d}x} + V(x) \psi = E \psi, \tag{22}$$

where $V(x) = A/(x + b/a) + Bx$. It is important to remark at this point that we fixed the ambiguity parameters as stated above, because we infer that the form of the potential should not change the choice of the ambiguity parameters, and those parameters were fixed when treating the free case in above. By making a translation ($x = y + b/a$), one can rewrite the above equation in the form

$$-y \frac{\mathrm{d}^2 \psi(y)}{\mathrm{d}y^2} - \frac{1}{a} \frac{\mathrm{d}\psi(y)}{\mathrm{d}x} + \left(\frac{\bar{A}}{y} - \bar{B} y \right) \psi(y) = \bar{E} \psi(y), \tag{23}$$

with $\bar{A} \equiv A/(\hbar^2 a)$, $\bar{B} \equiv B/(\hbar^2 a)$ and $\bar{E} \equiv (E + bB/a)/(\hbar^2 a)$. The above equation presents the following solution which is non-singular at the origin

$$\begin{aligned} \psi(y) = N y^g \, \mathrm{e}^{-\sqrt{\bar{B}} y}_1 F_1 &\left[\frac{1}{2} \left(-\frac{\bar{E}}{\sqrt{\bar{B}}} + \frac{1}{a} \sqrt{(a-1)^2 + 4\bar{A} a^2} + 1 \right); \right. \\ &\left. \frac{1}{a} \sqrt{(a-1)^2 + 4\bar{A} a^2} + 1; 2\sqrt{\bar{B}} y \right], \end{aligned} \tag{24}$$

where we defined that $g \equiv \frac{1}{2a}\left(\sqrt{(a-1)^2 + 4\bar{A}} + (a-1)\right)$, and N is a normalization constant. The requirement that the confluent hypergeometric function becomes a polynomial imposes the restriction which determines que quantization of the eigen-energies, so that

$$\frac{1}{2}\left(-\frac{\bar{E}}{\sqrt{\bar{B}}} + \frac{1}{a}\sqrt{(a-1)^2 + 4\bar{A}a^2} + 1\right) = -n, \tag{25}$$

and this leads us to the energy spectrum

$$E_n = \hbar\sqrt{\frac{B}{a}}\left((2n+1)a + \sqrt{(a-1)^2 + \frac{4A}{\hbar^2}}\right) - \frac{bB}{a}. \tag{26}$$

As an additional example, we could be tempted to include in the discussion a classical term like $pf(x)$. Unfortunately, however, it is unambiguous only in the coordinate representation, so that it ruins this property in the momentum one.

Finally, it is interesting to see that, in some very recent papers, it was adjudicated in favour of a Schroedinger equation in a phase-space representation, where appears a very interesting kind of mixing between the usual coordinate and momentum representations [35, 36]. It would be very interesting to see if this generalized representation could be useful in some particular problem, where there exists ordering ambiguity in both coordinate and momentum representations and maybe not in this new representation.

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