

Simple quantum systems in the momentum representation

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Abstract

The momentum representation is seldom used in quantum mechanics courses. Some students are thence surprised by the change in viewpoint when, in doing advanced work, they have to use the momentum rather than the coordinate representation. In this work, we give an introduction to quantum mechanics in momentum space, where the Schrödinger equation becomes an integral equation. To this end we discuss standard problems, namely, the free particle, the quantum motion under a constant potential, a particle interacting with a potential step, and the motion of a particle under a harmonic potential. What is not so standard is that they are all conceived from momentum space and hence they, with the exception of the free particle, are not equivalent to the coordinate space ones with the same names. All the problems are solved within the momentum representation making no reference to the systems they correspond to in the coordinate representation.

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1. Introduction

In quantum mechanics the spatial position, \hat{x} , and the linear momentum, \hat{p} , operators play very symmetrical roles, as it must be obvious from the fundamental commutation relation

$$[\hat{p}, \hat{x}] = \hat{p}\hat{x} - \hat{x}\hat{p} = -i\hbar \quad (1)$$

where, apart from a minus sign, the roles of \hat{x} and \hat{p} are the same. Notice that a hat over the symbols has been used to identify operators. However, this fundamental symmetry is not apparent to many students of quantum mechanics because an excessive emphasis is put on the coordinate representation in lectures and in textbooks. Some students are even lead to think of the coordinate space wave function $\psi(x)$ as more fundamental, in a certain way, than its momentum space counterpart $\phi(p)$; for, even in one of those rare cases where the Schrödinger equation is solved in momentum space, as is often the case with the linear potential x (Constantinescu and Magyari 1978), many students feel that the quantum solution is somewhat not complete until the coordinate space wave function has been found. This is a pity since a great deal of physical consequences are understood better and many physical effects are more readily evaluated in the momentum rather than in the coordinate representation; as an example just think of scattering processes and form factors of every kind (Taylor 1972, Ch 3; Frauenfelder and Henley 1974; Bransden and Joachaim 1983; Griffiths 1987). To give another interesting example, let us remember the one-dimensional hydrogen atom, an apparently simple system whose properties were finally understood, after thirty years of controversy (Loudon 1959, Elliot and Loudon 1960, Haines and Roberts 1969, Andrews 1976, Imbo and Sukhatme 1985, Boya *et al.* 1988, Núñez-Yépez *et al.* 1988, 1989, Martínez-y-Romero *et al.* 1989a,b,c) only after an analysis was carried out in the momentum representation (Núñez-Yépez *et al.* 1987, 1988, Davtyan *et al.* 1987).

But, besides particular occurrences, the advantages of an early introduction to the momentum representation in quantum mechanics are manyfold: a) to emphasize the basic symmetry between the representations, b) to introduce from the beginning and in a rather natural manner, distributions—pinpointing that the eigenfunctions are best regarded as generalized rather than ordinary functions—,

non-local operators and integral equations, c) to help clarify the different nature of operators in both representations, for example, in the momentum representation a free particle (vanishing potential in any representation) *cannot* be considered as equivalent to a particle acted by a constant (in momentum space) potential, since this last system admits a bound state. According to us the problems discussed in this work make clear, using rather simple examples, the distinct advantages and perhaps some of the disadvantages of working in the momentum representation.

2. Quantum mechanics in momentum space.

For calculating the basic properties and the stationary states of quantum mechanics systems, the fundamental equation is the time-independent Schrödinger equation which, in the coordinate representation, can be written as the differential eigenvalue equation

$$-\frac{\hbar^2}{2m} \frac{d^2\psi(x)}{dx^2} + U(x)\psi(x) = E\psi(x). \quad (2)$$

This can be obtained using, in the classical Hamiltonian $H = p^2/2m + U(x)$, the operator correspondence $\hat{p} \rightarrow -i\hbar d/dx$, $\hat{x} \rightarrow x$ [operators complying with (1)]. It is equally possible the use of the alternative operator correspondence $\hat{p} \rightarrow p$ and $\hat{x} \rightarrow i\hbar d/dp$ [also complying with (1)] that can be shown to lead —though not as straightforwardly as in the previous case— to the integral Schrödinger equation in the momentum representation

$$\frac{p^2}{2m}\phi(p) + \int dp' U(p-p')\phi(p') = E\phi(p), \quad (3)$$

where $U(p)$ is the Fourier transform of the potential energy function in the coordinate representation:

$$U(p) = \frac{1}{\sqrt{2\pi\hbar}} \int_{-\infty}^{+\infty} \exp(-ipx/\hbar) U(x) dx. \quad (4)$$

As it is obvious from (3), in this representation the potential energy becomes an integral operator (hence, usually non-local) in momentum space. Equations (2) and (3) are, in fact, Fourier transforms of each other; therefore the relationship between the coordinate and the momentum space wave functions is

$$\phi(p) = \frac{1}{2\pi\hbar} \int_{-\infty}^{+\infty} \exp(-ipx/\hbar) \psi(x) dx, \quad \text{and} \quad (5)$$

$$\psi(x) = \int_{-\infty}^{+\infty} \exp(+ipx/\hbar) \phi(p) dp.$$

Both functions, $\psi(x)$ and $\phi(p)$, characterize completely and independently the state of the system in question; although they differ slightly in interpretation: whereas $\psi(x)$ is the probability amplitude that a measurement of position gives a value in the interval $[x, x + dx]$, $\phi(p)$ is the probability amplitude that a measurement of momentum gives a value in the interval $[p, p + dp]$. It should be remarked that the normalization of a function in momentum space does not guarantee the normalization of the corresponding function in coordinate space, for this to be true you should multiply the transform of $\phi(p)$ times $\sqrt{2\pi\hbar}$.

In spite of their complete equivalence, the momentum representation could throw light in certain features that may remain hidden in the coordinate representation; very good examples of this are the SO(4) symmetry of the hydrogen atom first uncovered by Fock (1935) using his masterly treatment of the problem in the momentum representation; or the treatment of resonant Gamow states in the momentum representation where they were found to be, contrary to what happens in the coordinate representation, square integrable solutions to a homogeneous Lippmann-Schwinger equation (Hernández and Mondragón 1984).

In this work we calculate the bound energy eigenstates and corresponding quantum levels of the simplest one-dimensional potential problems in the momentum representation. We choose to present them in order of increasing complexity, as it is usually done in basic quantum mechanics:

- 1) The free particle with $U(p) = 0$.
- 2) Particle in a constant potential: $U(p) = -U_0$ ($U_0 > 0$).
- 3) Particle interacting with the potential step

$$U(p) = \begin{cases} 0, & \text{if } p > 0, \\ i\alpha \text{ } (\alpha \text{ a positive constant}), & \text{if } p \leq 0; \end{cases} \quad (6)$$

please notice that as we assume α to be a real number, the i factor is necessary to assure the Hermiticity of the potential energy operator.

4) Motion in the harmonic potential

$$U(p) = -f_0 \cos(ap), \quad (7)$$

where $f_0 > 0$ and a are real numbers.

As we intend to illustrate in this contribution, in many instances the eigenfunctions are easier to calculate in momentum space than in the coordinate space representation. We have to recognize though that the momentum space eigenstates are best understood as generalized functions or distributions—to which the Riemann interpretation of integrals does not apply; this is explicitly illustrated by examples A, B, and D below. The energy eigenvalues are calculated, in most cases discussed here (A, B, and D), as consistence conditions on the eigenfunctions, and in the remaining one, C, from the univaluedness of the eigenfunctions.

3. The examples.

We want to point out that albeit we are addressing the same type of systems that are used to introduce quantum mechanics, here we employ the same notion of simplicity but with problems posed in momentum space (making them very different from the coordinate space ones). Please be aware that we use atomic units wherever it is convenient in the rest of the paper: $\hbar = e = m = 1$.

A. The free particle.

In the case of the free particle, as in the coordinate representation, $U(p) = 0$ everywhere, so the Schrödinger equation (3) is simply

$$\left(\frac{p^2}{2} - E\right) \phi(p) = 0; \quad (8)$$

this deceptively simple equation has as its basic solutions

$$\phi_{p_E}(p) = A\delta(p - p_E) \quad (9)$$

where p_E is a solution of $p^2 = 2E$ and A is a constant. This is so since, according to (8), the wave function vanishes excepting when the energy takes its “on shell” value $E = p^2/2$; furthermore as $\phi(p)$ cannot vanish everywhere, equation (9) follows. The energy eigenfunctions (9) are also simultaneously eigenstates of the linear momentum,

$$\hat{p}\phi_{p_E}(p) = p\delta(p - p_E) = p_E\phi_{p_E}, \quad (10)$$

and form a generalized basis —*i.e.* formed by Dirac improper vectors— for the states of a free particle with well defined energy and linear momentum (Böhm 1979, Sakurai 1985); for such a free particle the most general stationary momentum-space solution is then

$$\Phi(p) = A_+\delta(p + |p_E|) + A_-\delta(p - |p_E|) \quad (11)$$

where the A_\pm are complex normalization constants; this solution represent a particle traveling to the right with momentum $|p_E|$ and to the left with momentum $-|p_E|$. The basic solutions (9) can be “orthonormalized” according to (Sakurai 1985)

$$\int_{-\infty}^{+\infty} \phi_{p_E}^*(p) \phi_{p'_E}(p) dp = \delta(p_E - p'_E) \quad (12)$$

which requires $A = 1$ in (9). The possible energy values are constrained only by the classical dispersion relation $E = p_E^2/2m$ hence they form a continuum and the eigenstates cannot be bound.

It is to be noted that for describing the eigenstates of a free particle, quantum mechanics uses generalized functions for which the probability densities $|\phi_{p_E}(p)|^2$ are not well defined! What it is well defined is their action on any square integrable function, hence on any physical state; therefore the eigenstates have to be regarded as linear functionals acting on $L^2(R)$, the set of all square integrable functions. The only physically meaningful way of dealing with free particles requires thus the use of wave packets as follows

$$\begin{aligned} \Phi(p) &= \int_{-\infty}^{+\infty} F(p') \delta(p - p') dp' \\ &= F(p), \end{aligned} \quad (13)$$

where $F(p)$ is any square integrable function of p . According to their properties then, improper vectors, like those in (9), though very useful for formal manipulations can never strictly represent physically realizable states (Taylor 1972, section 1a).

B. Motion under a constant potential

Substitution of the constant value $-U_0 < 0$ into (3), gives us

$$\left(\frac{p^2}{2} - E\right) \phi(p) = U_0 \int_{-\infty}^{+\infty} \phi(p') dp'; \quad (14)$$

to solve (14), let us define the number $\check{\varphi}$ as

$$\check{\varphi} \equiv \int_{-\infty}^{+\infty} \phi(p') dp'; \quad (15)$$

with this definition, the momentum representation Schrödinger equation (14) reduces to a purely algebraic equation for $\phi(p)$,

$$\left(\frac{p^2}{2} - E\right) \phi(p) = U_0 \check{\varphi}; \quad (16)$$

let us now define $k_0^2 = -2E > 0$, then the eigenfunctions are easily seen to be

$$\phi(p) = \frac{2U_0 \check{\varphi}}{p^2 + k_0^2}. \quad (17)$$

To determine the energy eigenvalues we integrate both sides of (17) from $-\infty$ to $+\infty$ to get

$$\check{\varphi} = -2\pi \frac{U_0 \check{\varphi}}{k_0} \quad \text{or} \quad E = -2\pi^2 U_0^2; \quad (18)$$

the system has a single energy eigenstate with the energy eigenvalue given in (18). The associated normalized eigenfunction is then

$$\phi(p) = \sqrt{\frac{2}{\pi}} \frac{k_0^{\frac{3}{2}}}{p^2 + k_0^2}. \quad (19)$$

It is important to emphasize what we have shown: a constant potential in momentum space admits a bound state. Obviously then in this representation we have not the freedom of changing the origin of the potential energy by adding a constant. *In momentum space the potential energy is undetermined not up to a constant value but up to a Dirac-delta function potential*; that is, if you take an arbitrary potential $U(p)$ in momentum space, the physics of the problem is not changed when you consider instead the modified potential $U'(p) = U(p) + \gamma \delta(p)$ with γ an arbitrary constant, whereas the change $U''(p) = U(p) + \gamma \neq U'(p)$ **does** indeed change the physics. The reader can prove by herself this elementary fact.

This discussion is going forward apparently with no trouble; we have to acknowledge though that for getting to the condition (18), we quickly passed over a very important point, the integral of the right hand side of (17) does not exist in the ordinary Riemann sense. To obtain our result you need to do it instead in the distribution sense, regarding the momentum space function $\phi(p)$ as a linear functional acting upon square integrable functions, as corresponds to possible state functions of a quantum system. Such idea is also behind the usefulness of the delta functions as generalized basis for the free particle states in example A.

To particularize to the present situation, this amounts to make $\hat{\varphi}$ convergent (hence meaningful) when acting on any state function (Richtmyer 1978, Böhm 1979). A direct way of accomplishing this is, as usually done in theoretical physics (Taylor 1972, Frauenfelder and Henley 1974, Griffiths 1987), to get the mentioned integral come into existence in a principal value sense (Mathews and Walker 1970). To this end first multiply the right hand side of (17) times an $\exp(-i\epsilon p)$ complex factor, then perform the integral using contour integration in the complex plane and, *at the very end*, take the limit $\epsilon \rightarrow 0$. With such provisos considered, it is not difficult getting the result (18). However, this means that the functions involved in our discussion have to be considered as linear functionals or generalized functions, as can be done—perhaps it would be better to say: *should be done*—for every wave function of a quantum system (Messiah 1976, Böhm 1979); forgetting this fact can produce erroneous results as it is exemplified by the case discussed in (Núñez-Yépez and Salas-Brito 1987).

It is to be noted that the free particle potential acts as a confining potential in momentum space; it allows, for each—out of a nonnegative continuum—energy value, just two choices for the momentum: $|p_E|$ and $-|p_E|$; such extreme restriction is also reflected in the wave functions, they are Dirac delta functions which peak at the just quoted values of p . On the other hand, the constant potential, which does not restrict the possible values of the momentum in the severe way of the zero potential, is not as confining in momentum space and allows a single energy eigenvalue whose associated eigenstate requires a very wide range of momenta [given in (19)] to exist. At this point we invite the reader to try to solve the problem of a particle inside an infinite potential box—in *momentum space*. This is a simple and nice exercise to test the intuition on the differences between the

momentum and the coordinate representation; it is not difficult to conclude that, in this case, the eigenfunctions are also Dirac delta functions with a lightly but subtly modified relation linking energy and momentum.

C. Motion in a potential step

In this case $U(p)$ is given in (6). Using such potential, the Schrödinger equation becomes a simple Volterra integral equation

$$\left(\frac{p^2}{2} - E\right) \phi(p) + i\alpha \int_{-\infty}^p \phi(p') dp'. \quad (20)$$

To solve this equation, we derive both members and, using $k_0^2 \equiv -2E$, we obtain a very simple differential equation

$$\frac{d\phi(p)}{dp} = 2 \frac{p - i\alpha}{p^2 + k_0^2} \phi(p), \quad (21)$$

whose solution is

$$\phi_{k_0}(p) = \frac{A}{p^2 + k_0^2} \left[\frac{k_0 - ip}{k_0 + ip} \right]^{\alpha/k_0} \quad (22)$$

with A an integration constant.

The energy eigenvalues follow, not from a consistency condition as in the last example, B, but from the requirement that the eigenfunctions be single valued. This is only possible if α/k_0 takes nonnegative integer values (Churchill 1960), *i.e.* if $k_0 = \alpha/n$, $n = 1, 2, \dots$, the value $n = 0$ is not allowed for $\phi(p)$ would vanish identically in that case (Núñez-Yépez *et al.* 1987). Thus, the system has an infinite number of bound energy eigenstates with energies given by

$$E_n = -\frac{\alpha^2}{2n^2}, \quad n = 1, 2, \dots; \quad (23)$$

the normalization of the eigenfunctions requires that $A = (2\alpha^3/n^3\pi)^{1/2}$ in equation (22).

A very important property of the eigenfunctions is

$$\int_{-\infty}^{+\infty} \phi(p) dp = 0, \quad (24)$$

this is required to guarantee the Hermiticity of the Hamiltonian operator of the problem (Andrews 1976, Núñez-Yépez *et al.* 1987, Salas-Brito 1990). We pinpoint

that the potential step in momentum space is particularly interesting because it is closely related to the study of the momentum space behaviour of electrons interacting with the surface of liquid helium, with the properties of the an hydrogen atom in superstrong magnetic fields, and with certain supersymmetric problems (Cole and Cohen 1969, Imbo and Sukhatme 1985, Núñez-Yépez *et al.* 1987, Martínez-y-Romero *et al.* 1989c, Salas-Brito 1990).

D. Motion under a harmonic potential

Let us, as our final example, study the motion of a particle under the harmonic potential $U(p) = -f_0 \cos(ap)$, where a and $f_0 > 0$ are real constants. The Schrödinger equation is then

$$\frac{p^2}{2}\phi(p) - f_0 \int_{-\infty}^{+\infty} \cos[a(p-p')] \phi(p') dp' = E\phi(p). \quad (25)$$

By changing p for $-p$ in (25) we can show that the Hamiltonian commutes with the parity operator, thus its eigenfunctions can be chosen as even or odd functions, *i.e.* as parity eigenstates.

For solving (25), let us define $k^2 \equiv -2E$ and, using the identity $2\cos x = \exp(ix) + \exp(-ix)$, we easily obtain the eigenfunctions as

$$\phi(p) = \frac{2f_0}{p^2 + k^2} [\check{\varphi}_+ e^{-iap} + \check{\varphi}_- e^{iap}], \quad (26)$$

where the numbers $\check{\varphi}_{\pm}$ are defined by

$$\check{\varphi}_{\pm} \equiv \int_{-\infty}^{+\infty} e^{\pm iap'} \phi(p') dp'. \quad (27)$$

As in the constant potential (example B), the energy eigenvalues follow from using the definitions (27) back in the eigenfunctions (26)—please remember that we require the functions (26) be regarded as in example B, for doing the integrals (27). The integrals gives us the following two conditions

$$\begin{aligned} \check{\varphi}_+ &= \frac{2f_0\pi}{k} [\check{\varphi}_+ + \check{\varphi}_- \exp(-2ak)], \\ \check{\varphi}_- &= \frac{2f_0\pi}{k} [\check{\varphi}_- + \check{\varphi}_+ \exp(+2ak)]. \end{aligned} \quad (28)$$

As the eigenfunctions can be chosen as even or odd, we can select the numbers $\check{\varphi}_{\pm}$ to comply with $\check{\varphi}_+ = \pm \check{\varphi}_-$, so the eigenfunctions are

$$\begin{aligned}\phi_+(p) &= \frac{A_+}{p^2 + k^2} \cos(ap), \\ \phi_-(p) &= \frac{A_-}{p^2 + k^2} \sin(ap);\end{aligned}\tag{29}$$

which correspond to the complete set of eigenfunctions of the problem.

From (28) we also get the two equations determining the energy eigenvalues

$$\frac{k}{2f_0\pi} - 1 = \pm e^{-2ak}.\tag{30}$$

one for the odd and the other for the even state. As can be seen in Figure 1, in general equations (30) admits two solutions, let us call them k_+ (for the even state) and k_- (for the odd state). Therefore the system has a maximum of two eigenvalues $E_+ = -k_+^2/2$ and $E_- = -k_-^2/2$; the ground state is always even and the excited (odd) state exist only if $f_0 \leq f_0^{\text{crit}} = 1/4a\pi \simeq 0.0796$.

The analysis is easily done using the graph shown in Figure 1, where we plot together $-\alpha k + 1$, $\alpha k - 1$ and $\exp(-2ak)$ [using $\alpha \equiv 1/(2f_0\pi) = 1$] against k , for illustrating the roots of (30). In the plot, we have used the values $a = 1$, $f_0 = 1/2\pi \simeq 0.1592$, corresponding to the roots $k_- = 0.7968$ (the leftmost root) and $k_+ \simeq 1.109$ (the rightmost root); thus the energy eigenvalues are $E_+ \simeq -0.6148$ (the ground state) and $E_- \simeq -0.3175$ (the excited state). The criterion for the existence of the excited state and the value for f_0^{crit} follows from Figure 1, by noting that such critical value stems from the equality of the slopes of the two curves meeting at the point $(0, 1)$ in the plot. Notice also that the results previously obtained for the constant potential (example B) can be recovered as a limiting case of the harmonic potential if we let $a \rightarrow 0$.

4. Concluding remarks

We have discussed four instructive one-dimensional examples in quantum mechanics from the point of view of momentum space. Purportedly we have not made any reference to the problems they represent in the coordinate representation. We expect to contribute with our approach to the development of physical insight for problems posed in the momentum representation and, furthermore, to help students to understand the different features of operators, as opposed to classical variables, in different representations. We also expect to made clear that sometimes it is better to treat a problem from the momentum space point of view since

the solution can be simplified. The point at hand is the simple form in which the momentum space eigenfunctions are obtained in the problems discussed here; though these have to be regarded as distributions for obtaining the associated energy eigenvalues.

With goals as the mentioned in mind and to point out other advantages of the momentum representation, in a formal set of lectures and depending on the level of the students, it may be also convenient to discuss more complex problems: as scattering and dispersion relations (Taylor 1972), or the study of resonant states as solutions of a Lippmann-Schwinger equation in momentum space (Hernández and Mondragón 1984), or the 3D hydrogen atom, whose solution using Fock's method is nicely exposed in (Bransden and Joachaim 1983).

Just in the case you are wondering and have not found the time for doing the transformations yourself, let us say that the problems, save the free particle, we have posed and solved in this paper are known, in the coordinate representation, as 1) the attractive delta potential (Example B), 2) quantum motion under the (quasi-Coulomb) potential $1/x$ (Example C) and, finally, the problem of two equal (intensity: $A = -\pi f_0/\sqrt{2}$), symmetrically placed, attractive delta function potentials, which are displaced by $2a$ from one another (Example D).

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Figure Caption

Figure 1

The figure illustrates the solution to equations (30) determining the energy eigenvalues under the harmonic potential (7). We here plot $\exp(-2ak)$, $\alpha k - 1$ and $-\alpha k + 1$ against k all in the same graph. Just for illustration purposes, we have used the specific values $a = 1$, $f_0 = 1/2\alpha\pi \simeq 0.1592$, (we have defined $\alpha = 1/2f_0\pi$ and used $\alpha = 1$). The critical value of f_0 , giving birth to the excited state, is $f_0^{\text{crit}} = (4a\pi)^{-1}$ as can be obtained from the equality of the slopes of the two curves meeting at the point $(0, 1)$ in the graph. In the situation exemplified by this figure, $f_0^{\text{crit}} \simeq 0.0796$ and the roots of equations (30) are $k_+ \simeq 1.109$ and $k_- \simeq 0.7968$.

