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Quantum mechanical time-development operator for the uniformly accelerated particle*

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Abstract

We derive a useful expression for the time-development operator for quantum wavefunctions, $\exp(-i\hat{H}t/\hbar)$, for the case of a particle subject to a constant force. We apply it, in both position- and momentum-space, to construct wavepackets which exhibit uniform acceleration. We use these results to generate quantum wavepackets corresponding to the motion of a charged particle in a uniform electric field in two different gauges, explicitly demonstrating the change in phase of the wavefunction under a gauge transformation. The more standard description of the time-dependence of accelerating wavepackets using the formalism of propagators is briefly reviewed in an appendix for comparison.

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I. Introduction

While many elementary textbooks on quantum mechanics focus on the solution of the time-independent Schrödinger equation, solving for energy eigenstates, the study of the time-dependence of a general quantum state is also of great importance. The time-evolution of such a state can be described via the Schrödinger equation, namely

$$\hat{H}|\psi\rangle_t = i\hbar \frac{\partial}{\partial t}|\psi\rangle_t \quad (1)$$

where $\hat{H}$ is the appropriate Hamiltonian operator and $|\psi\rangle$ can be a position-space ($\psi(x, t)$) or momentum-space ($\phi(p, t)$) wavefunction or given by a matrix representation.

In any case, Eqn. 1 can be *formally* solved by direct integration to give the familiar relation

$$|\psi\rangle_t = e^{-i\hat{H}t/\hbar}|\psi\rangle_0 \quad (2)$$

assuming that $\hat{H}$ is itself independent of time. This approach can be very useful in a variety of formal applications such as investigating the connections between unitary operators and conservation of probability, the relation between the Schrödinger and Heisenberg pictures, and the time-development of expectation values of operators and their relation to conservation laws. On the more ‘applied’ side, Eqn. 2 can be approximated and discretized appropriately to provide numerical solutions for time-dependent scattering problems in one [1] and two [2] dimensions.

Given the utility of this formulation of the time-development of a quantum state, it is perhaps disappointing that there are so few examples in which Eqn. 2 can be applied to a given initial state to yield closed-form solutions representing wavepackets. Blinder [3] has shown how Eqn. 2 can be applied, in the free particle case, to an

initial Gaussian position-space wavefunction to generate standard spreading Gaussian wavepackets. (One must be cautious, however, in the application of his method to more general initial states as noted by Holstein and Swift [4].) The main purpose of this note is to provide another set of similar examples, this time corresponding to the quantum mechanical problem of a particle subject to a constant force, in which the time-development operator can also be used to generate closed-form wavepacket solutions. We are especially interested in using such methods to evaluate the time-dependence of momentum-space wavefunctions which further extends the work of Ref. [3] in a complementary way.

In Sec. II, we very briefly review free-particle Gaussian wavepackets, in both position- and momentum-space, as obtained from a Schrödinger equation approach, as well as the application of Eqn. 2 to yield the same results; this will also help establish notation. In Sec. III, we obtain wavepacket solutions in both x - and p -space using the Schrödinger equation for a particle subjected to a uniform force, while in Sec. IV we obtain these same results by the use of Eqn. 2, supplemented by an important operator identity. Finally, in Sec. V, we apply some of these same techniques to discuss wavepacket solutions which describe the motion of a charged particle in a uniform electric field. We will generate such solutions in two different gauges and thus be able to confirm explicitly the appropriate phase relation between them as required by gauge invariance. For completeness, an appendix reviews the more standardly used propagator approach to the quantum problem of a particle under a constant force for comparison to the methods described here.

II. Free-particle time-development operator and wavepackets

The free-particle Schrödinger equation in position-space, namely

$$-\frac{\hbar^2}{2m} \frac{\partial^2 \psi(x, t)}{dx^2} = i\hbar \frac{\partial \psi(x, t)}{\partial t} \quad (3)$$

can be rewritten in momentum-space by using the standard Fourier transform connections

$$\phi(p, t) = \frac{1}{\sqrt{2\pi\hbar}} \int_{-\infty}^{+\infty} \psi(x, t) e^{-ipx/\hbar} dx \quad (4)$$

$$\Updownarrow$$

$$\psi(x, t) = \frac{1}{\sqrt{2\pi\hbar}} \int_{-\infty}^{+\infty} \phi(p, t) e^{ipx/\hbar} dp \quad (5)$$

in the form

$$\frac{p^2}{2m} \phi(p, t) = i\hbar \frac{\partial \phi(p, t)}{\partial t} \quad (6)$$

The time-dependence of $\phi(p)$ is then trivially obtained to be

$$\phi(p, t) = \phi(p, 0) e^{-ip^2 t/2m\hbar} = \phi_0(p) e^{-ip^2 t/2m\hbar} \quad (7)$$

so that the momentum-space probability does not vary with time since

$$|\phi(p, t)|^2 = |\phi(p, 0)|^2 = |\phi_0(p)|^2 \quad (8)$$

The familiar Gaussian wavepacket in position-space can be obtained by choosing the momentum-space wavefunction

$$\phi_0(p) = \sqrt{\frac{\alpha}{\sqrt{\pi}}} e^{-\alpha^2 p^2/2} \quad (9)$$

which has $\Delta p = 1/\alpha\sqrt{2}$. This can be integrated using Eqn. 5 and standard integrals such as

$$\int_{-\infty}^{+\infty} e^{-ax^2-bx} dx = \sqrt{\frac{\pi}{a}} e^{b^2/4a} \quad (10)$$

to give

$$\psi(x, t) = \frac{1}{\sqrt{\alpha\hbar\sqrt{\pi}(1 + it/t_0)}} \exp\left[-\frac{x^2}{2\alpha^2\hbar^2(1 + it/t_0)}\right] \quad (11)$$

where $t_0 = m\hbar\alpha^2$ is associated with a spreading time. The position-space probability density is then

$$|\psi(x, t)|^2 = \frac{1}{\beta_t\sqrt{\pi}} e^{-x^2/\beta_t^2} \quad (12)$$

where

$$\beta_t = \alpha\hbar\sqrt{1 + \frac{t^2}{t_0^2}} = \beta\sqrt{1 + t^2/t_0^2} \quad (13)$$

and $\Delta x = \beta_t/\sqrt{2}$ so that the position-space wavepacket spreads in time. A more general $\psi(x, t)$, with arbitrary initial position and average momenta given by x_0 and p_0 , is easily obtained by the substitution

$$\phi_0(p) \longrightarrow \phi_0(p - p_0) e^{-ipx_0/\hbar} \quad (14)$$

These same results can be obtained by using the time-development operator in Eqn. 2. In the momentum-space representation, the Hamiltonian is simply the kinetic energy, i.e.,

$$\hat{H} = \frac{p^2}{2m} \quad (15)$$

so that

$$\phi(p, t) = e^{-i\hat{H}t/\hbar} \phi(p, 0) = e^{-ip^2 t/2m\hbar} \phi(p, 0) \quad (16)$$

just as in Eqn. 7. On the other hand, in position space, the kinetic energy operator is non-trivial and given by

$$\hat{H} = \frac{\hat{p}^2}{2m} = -\frac{\hbar^2}{2m} \frac{d^2}{dx^2} \quad (17)$$

so that the time-development operator is

$$e^{-i\hat{H}t/\hbar} = \exp\left[i\frac{\hbar t}{2m} \left(\frac{\partial^2}{\partial x^2}\right)\right] \quad (18)$$

Blinder [3] noted that the time-development operator could be applied to the initial wavefunction

$$\psi(x, 0) = \frac{1}{\sqrt{\beta}\sqrt{\pi}} e^{-x^2/2\beta^2} \equiv \sqrt{\frac{\beta}{2\sqrt{\pi}}} \left[w^{-1/2} e^{-x^2/4w} \right] \quad (19)$$

where $2w = \beta^2$, to obtain a closed form result for $\psi(x, t)$. His proof relied on the useful identity

$$\frac{\partial^2}{\partial x^2} \left[w^{-1/2} e^{-x^2/4w} \right] = \frac{\partial}{\partial w} \left[w^{-1/2} e^{-x^2/4w} \right] \quad (20)$$

which implies that

$$\begin{aligned} \psi(x, t) &= \exp \left[-i \frac{\hat{H}t}{\hbar} \right] \psi(x, 0) \\ &= \exp \left[i \left(\frac{\hbar t}{2m} \right) \left(\frac{\partial^2}{\partial x^2} \right) \right] \left\{ \sqrt{\frac{\beta}{2\sqrt{\pi}}} \left[w^{-1/2} e^{-x^2/4w} \right] \right\} \\ &= \sqrt{\frac{\beta}{2\sqrt{\pi}}} \exp \left[i \left(\frac{\hbar t}{2m} \right) \left(\frac{\partial}{\partial w} \right) \right] \left\{ w^{-1/2} e^{-x^2/4w} \right\} \\ &= \sqrt{\frac{\beta}{2\sqrt{\pi}}} \frac{1}{\sqrt{w + i\hbar t/2m}} \exp \left[-\frac{x^2}{4(w + i\hbar t/2m)} \right] \\ \psi(x, t) &= \frac{1}{\sqrt{\beta}\sqrt{\pi}(1 + it/t_0)} \exp \left[-\frac{x^2}{2\beta^2(1 + it/t_0)} \right] \end{aligned} \quad (21)$$

We have used the fact that the exponential of a single derivative operator can be written in terms of a generalized translation, i.e.,

$$\exp \left[a \frac{\partial}{\partial w} \right] f(w) = f(w + a) \quad (22)$$

which can be easily proved by expanding the exponential as a power series and comparing to the Taylor series for $f(z + a)$, expanded around z .

III. Wavepackets for uniformly accelerating particle via the Schrödinger equation

For a particle subject to a constant force in the positive x -direction, the potential energy function is given by $V(x) = -Fx$ so that the Hamiltonian operator can be written as

$$\hat{H}_F = \frac{p^2}{2m} - Fx \quad (23)$$

We do not explicitly denote either p or x as operators as we will work in both representations. As is well known, the resulting time-dependent Schrödinger equation

$$-\frac{\hbar^2}{2m} \frac{\partial^2 \psi(x, t)}{dx^2} - Fx\psi(x, t) = i\hbar \frac{\partial \psi(x, t)}{\partial t} \quad (24)$$

can be solved for energy eigenstates with corresponding Airy function solutions. The resulting position-space solutions can be used to formally construct wavepacket-type solutions [5] or more directly used for comparison with classical probability distributions [6] to exhibit the expected uniform acceleration. (We note that we are not discussing solutions related to the ‘nonspreading wavepackets’ in the form of an Airy function discussed by Berry and Balazs [7] and Greenberger [8].) Because this problem is most often discussed in terms of propagator methods, for completeness, we briefly review that approach in the appendix for comparison.

In order to construct more useful, closed-form wavepackets, we choose first to work in momentum-space where the time-dependent Schrödinger equation becomes

$$\frac{p^2}{2m} \phi(p, t) - i\hbar F \frac{\partial \phi(p, t)}{\partial p} = i\hbar \frac{\partial \phi(p, t)}{\partial t} \quad (25)$$

This can be rewritten in the form

$$i\hbar \left(F \frac{\partial \phi(p, t)}{\partial p} + \frac{\partial \phi(p, t)}{\partial t} \right) = \frac{p^2}{2m} \phi(p, t) \quad (26)$$

which emphasizes the fact that any function of the combination $p - Ft$ will make the left-side vanish. Motivated by this, we attempt a solution of the form

$$\phi(p, t) = \Phi(p - Ft)\tilde{\phi}(p) \quad (27)$$

which implies that $\tilde{\phi}(p)$ must satisfy

$$\frac{d\tilde{\phi}(p)}{dp} = -\frac{ip^2}{2m\hbar F}\tilde{\phi}(p) \quad (28)$$

which gives

$$\tilde{\phi}(p) = e^{-ip^3/6m\hbar F} \quad (29)$$

A general solution which reduces to a given initial momentum-space amplitude, $\phi_0(p)$ can then be written in the form

$$\begin{aligned} \phi(p, t) &= \phi_0(p - Ft)e^{i((p - Ft)^3 - p^3)/6m\hbar F} \\ &= \phi_0(p - Ft) \exp \left[-\frac{ip^2 t}{2m\hbar} + \frac{ipFt^2}{2m\hbar} - \frac{iF^2 t^3}{6m\hbar} \right] \end{aligned} \quad (30)$$

where we have used $\Phi(p - Ft) = \phi_0(p - Ft) \exp(i(p - Ft)^3/6m\hbar F)$. The solution in Eqn. 30 obviously satisfies

$$|\phi(p, t)|^2 = |\phi_0(p - Ft)|^2 \quad (31)$$

and gives $\langle p \rangle_t = \langle p \rangle_0 + Ft$ corresponding to a uniform ‘translation’ of the momentum-space probability density consistent with a constant force. The ‘spread’ in momentum stays fixed since $\Delta p_t = 1/\sqrt{2}\alpha$. The average value of position can be calculated quite generally using the identification

$$x \longrightarrow \hat{x} = i\hbar \frac{\partial}{\partial p} \quad (32)$$

so that

$$\begin{aligned}
\langle \hat{x} \rangle_t &= \int_{-\infty}^{+\infty} dp \phi^*(p, t) \left(i\hbar \frac{\partial}{\partial p} \right) \phi(p, t) \\
&= \int_{-\infty}^{+\infty} \phi_0^*(p - Ft) \left(i\hbar \frac{\partial}{\partial p} \right) \phi_0(p - Ft) \\
&\quad + \frac{t}{m} \int_{-\infty}^{+\infty} |\phi_0(p - Ft)|^2 p dp - \frac{Ft^2}{2m} \int_{-\infty}^{+\infty} |\phi_0(p - Ft)|^2 dp \\
&= \langle \hat{x} \rangle_0 + \frac{t}{m} \langle p \rangle_0 + \frac{Ft^2}{2m}
\end{aligned} \tag{33}$$

where

$$\langle \hat{x} \rangle_0 = \int_{-\infty}^{+\infty} \phi_0(p) \left(i\hbar \frac{\partial}{\partial p} \right) \phi_0(p) \quad \text{and} \quad \langle p \rangle_0 = \int_{-\infty}^{+\infty} |\phi_0(p)|^2 p dp \tag{34}$$

and simple changes of variables are used to bring the terms in Eqn. 33 into these forms.

Because the exponential factor in Eqn. 30 is quadratic, one can still find the corresponding $\psi(x, t)$ using a Gaussian initial $\phi_0(p)$ of the form in Eqn. 9. The result is then

$$\begin{aligned}
\psi(x, t) &= \frac{1}{\sqrt{\alpha\hbar\sqrt{\pi}(1 + it/t_0)}} \exp \left[\frac{iFt}{\hbar} \left(x - \frac{Ft^2}{6m} \right) \right] \\
&\quad \times \exp \left[-\frac{(x - Ft^2/2m)^2}{2\hbar^2\alpha^2(1 + it/t_0)} \right]
\end{aligned} \tag{35}$$

with the corresponding position-space probability density

$$|\psi(x, t)|^2 = \frac{1}{\beta_t \sqrt{\pi}} e^{-(x - Ft^2/2m)^2 / \beta_t^2} \tag{36}$$

This can be easily seen to correspond to uniformly accelerated motion with

$$\langle x \rangle_t = \frac{Ft^2}{2m} = \frac{1}{2}at^2 \tag{37}$$

while $\Delta x_t = \beta_t / \sqrt{2}$, so it spreads in the same manner as the more frequently discussed free-particle Gaussian wavepacket. For completeness, we note that it is easy to show

(in either representation) that the expectation values of the energy, kinetic energy, and potential energy for this Gaussian state are given by

$$\langle \hat{E} \rangle_t = \frac{1}{4m\alpha^2} \quad \langle V(x) \rangle_t = -\frac{F^2 t^2}{2m} \quad \langle \hat{T} \rangle_t = \left\langle \frac{p^2}{2m} \right\rangle_t = \frac{1}{4m\alpha^2} + \frac{F^2 t^2}{2m} \quad (38)$$

which can be discussed in terms of their classical counterparts for uniformly accelerated motion.

IV. Time-development operator for a particle subject to a constant force

In order to obtain similar results using the time-development operator, $\exp(-i\hat{H}_F t/\hbar)$, we first recall the identity, sometimes described as the Campbell-Baker-Hausdorff formula, relating the exponentials of operators, namely

$$e^{\hat{A}} e^{\hat{B}} = e^{\hat{O}} \quad (39)$$

where

$$\begin{aligned} \hat{O} = & \hat{A} + \hat{B} + \frac{1}{2} [\hat{A}, \hat{B}] + \frac{1}{12} ([[\hat{A}, \hat{B}], \hat{B}] + [\hat{A}, [\hat{A}, \hat{B}]]) \\ & + \frac{1}{24} ([[[\hat{B}, \hat{A}], \hat{A}], \hat{B}] + \dots \end{aligned} \quad (40)$$

Simplified versions of this relation are often discussed in textbooks [9] in the special case where the commutator $[\hat{A}, \hat{B}]$ commutes with $\hat{A}$ and $\hat{B}$ so that the double-commutators and higher terms vanish. The general case above is nicely demonstrated by Weiss and Maradudin [10] who also give references to the early studies of Campbell and Baker and the original proof by Hausdorff.

To make use of this relation, we first let

$$\hat{A} = -\frac{i\hat{H}_F t}{\hbar} = -\frac{it}{\hbar} \left(\frac{p^2}{2m} - Fx \right) \quad (41)$$

and

$$\hat{B} = -\frac{it}{\hbar} (Fx) \quad (42)$$

so that

$$\hat{A} + \hat{B} = -\frac{ip^2 t}{2m\hbar} \quad (43)$$

Using the basic commutation relation between x and p , the various commutators in Eqn. 40 are given by

$$[\hat{A}, \hat{B}] = \frac{iFt^2}{m\hbar} p \quad (44)$$

$$[[\hat{A}, \hat{B}], \hat{B}] = -\frac{iF^2 t^3}{m\hbar} = [\hat{A}, [\hat{A}, \hat{B}]] \quad (45)$$

and all higher commutators vanish. If we multiply Eqn. 39 on the right by the operator $e^{-\hat{B}}$, we can write

$$e^{\hat{A}} = e^{\hat{O}} e^{-\hat{B}} \quad \Rightarrow \quad e^{-i\hat{H}_F t/\hbar} = \exp \left[-\frac{ip^2 t}{2m\hbar} + \frac{iFt^2 p}{2m\hbar} - \frac{iF^2 t^3}{6m\hbar} \right] e^{iFtx/\hbar} \quad (46)$$

In a position-space representation, the position coordinate x is represented by a non-trivial operator, namely $\hat{x} = i\hbar(\partial/\partial p)$; this implies that

$$\exp \left(\frac{iFt\hat{x}}{\hbar} \right) g(p) = \exp \left(-Ft \frac{\partial}{\partial p} \right) g(p) = g(p - Ft) \quad (47)$$

generalizing Eqn. 22. For momentum-space wavefunctions, we then have the time-dependent solution

$$\begin{aligned} \phi(p, t) &= e^{-i\hat{H}_F t/\hbar} \phi(p, 0) \\ &= e^{-i\hat{H}_F t/\hbar} \phi_0(p) \\ &= \exp \left[-\frac{ip^2 t}{2m\hbar} + \frac{iFt^2 p}{2m\hbar} - \frac{iF^2 t^3}{6m\hbar} \right] \phi_0(p - Ft) \end{aligned} \quad (48)$$

just as in Eqn. 30.

The time-development operator for the position-space wavefunction is more conveniently written by interchanging the definitions of the operators $\hat{A}$ and $\hat{B}$ in Eqns. 41 and 42 and considering the exponential operator identity in the form

$$e^{\hat{B}} = e^{-\hat{A}} e^{\hat{O}} \quad (49)$$

obtained by multiplying Eqn. 40 by the inverse of $\exp(\hat{A})$, this time on the left. The appropriate expression is now

$$\begin{aligned} e^{-i\hat{H}_F t/\hbar} &= e^{iFtx/\hbar} \exp \left[-\frac{i\hat{p}^2 t}{2m\hbar} - \frac{iFt^2 \hat{p}}{2m\hbar} - \frac{iF^2 t^3}{6m\hbar} \right] \\ &= e^{iFt(x-Ft^2/6m)/\hbar} \exp \left[-\frac{i\hat{p}^2 t}{2m\hbar} \right] \exp \left[-\frac{iFt^2 \hat{p}}{2m\hbar} \right] \end{aligned} \quad (50)$$

where we have specialized to position space where $\hat{p} = (\hbar/i)(\partial/\partial x)$ is the differential operator. We have also used the fact that the operator $\hat{p}$ can be freely ‘moved around’ inside the exponentials as any power of an operator commutes with itself and Eqn. 40 simplifies. The effect of the right-most exponential operator in Eqn. 50 is given by

$$\exp \left[-\frac{iFt^2 \hat{p}}{2m\hbar} \right] f(x) = \exp \left[-\frac{Ft^2}{2m} \frac{\partial}{\partial x} \right] f(x) = f \left(x - \frac{Ft^2}{2m} \right) \quad (51)$$

which once again generalizes the result of Eqn. 22, in a different way. The remaining operator is simply the free-particle time-development operator which, for an initial Gaussian position-space amplitude, explicitly induces the time-spreading of the width. Therefore, the net effect of Eqn. 50 on such an initial Gaussian is

$$\begin{aligned} \psi(x, t) &= e^{-i\hat{H}_F t/\hbar} \psi(x, 0) \\ &= e^{-i\hat{H}_F t/\hbar} \left[\frac{1}{\sqrt{\beta\sqrt{\pi}}} e^{-x^2/2\beta^2} \right] \end{aligned}$$

$$\begin{aligned}
&= \exp \left[\frac{iFt}{\hbar} \left(x - \frac{Ft^2}{6m} \right) \right] e^{-i\hat{p}^2 t / 2m\hbar} \left[\frac{1}{\sqrt{\beta\hbar}\sqrt{\pi}} e^{-(x - Ft^2/2m)^2 / 2\beta^2} \right] \quad (52) \\
&= \frac{1}{\sqrt{\beta\hbar}\sqrt{\pi}(1 + it/t_0)} \exp \left[\frac{iFt}{\hbar} \left(x - \frac{Ft^2}{6m} \right) \right] \\
&\quad \times \exp \left[-\frac{(x - Ft^2/2m)^2}{2\beta^2(1 + it/t_0)} \right]
\end{aligned}$$

just as in Eqn. 35, where now $\alpha\hbar = \beta$.

We can also evaluate the expectation value of position for a general initial state by writing

$$|\psi\rangle_t = e^{-i\hat{H}_F t/\hbar} |\psi\rangle_0 \quad (53)$$

and its complex conjugate which gives

$$\langle x \rangle_t = \langle \psi_0 | e^{+i\hat{H}_F t/\hbar} x e^{-i\hat{H}_F t/\hbar} | \psi_0 \rangle = \langle \psi_0 | e^{\hat{O}} x e^{-\hat{O}} | \psi_0 \rangle \quad (54)$$

where

$$\hat{O} = \frac{i\hat{p}^2 t}{2m\hbar} + \frac{iFt^2\hat{p}}{2m\hbar} \quad (55)$$

as we have canceled exponential terms which obviously commute with x . The product in Eqn. 54 can be evaluated using the more familiar operator identity

$$e^{\hat{A}} \hat{B} e^{-\hat{A}} = \hat{B} + [\hat{A}, \hat{B}] + \frac{1}{2} [\hat{A}, [\hat{A}, \hat{B}]] + \frac{1}{3!} [\hat{A}, [\hat{A}, [\hat{A}, \hat{B}]]] + \dots \quad (56)$$

Identifying $\hat{A} = \hat{O}$ and $\hat{B} = x$, we find

$$\begin{aligned}
\langle x \rangle_t &= \langle \psi_0 | x | \psi_0 \rangle + \frac{t}{m} \langle \psi_0 | \hat{p} | \psi_0 \rangle + \frac{Ft^2}{2m} \langle \psi_0 | \psi_0 \rangle \\
&= \langle x \rangle_0 + \frac{t}{m} \langle \hat{p} \rangle_0 + \frac{Ft^2}{2m} \quad (57)
\end{aligned}$$

as expected.

V. Application to charged particle motion in a uniform electric field in different gauges.

The problem of a particle of charge q in a uniform electric field E in one-dimension is formally identical to the constant force problems considered in Secs. III and IV since the potential is given by $V(x) = q\phi(x) = -qEx = -Fx$ where we will henceforth identify $F = qE$. Problems involving electromagnetism, however, have a richer structure as many sets of vector and scalar potentials can give rise to the same field strengths via the definitions

$$\mathbf{E}(\mathbf{r}, t) = -\nabla\phi(\mathbf{r}, t) - \frac{\partial}{\partial t}\mathbf{A}(\mathbf{r}, t) \quad \mathbf{B}(\mathbf{r}, t) = \nabla \times \mathbf{A}(\mathbf{r}, t) \quad (58)$$

Sets of $\mathbf{A}$ and ϕ which are related by a gauge transformation of the form

$$\mathbf{A}'(\mathbf{r}, t) = \mathbf{A}(\mathbf{r}, t) + \nabla f(\mathbf{r}, t) \quad (59)$$

$$\phi'(\mathbf{r}, t) = \phi(\mathbf{r}, t) - \frac{\partial}{\partial t}f(\mathbf{r}, t) \quad (60)$$

give rise to the same observable fields and hence to the same physics; we will describe $f(\mathbf{r}, t)$ as the gauge function.

The electromagnetic potentials arise in quantum mechanics via their incorporation into the Hamiltonian via

$$\hat{H} = \frac{1}{2m} (\hat{\mathbf{p}} - q\mathbf{A})^2 + q\phi \quad (61)$$

Under a gauge transformation, the Hamiltonian changes form to

$$\hat{H}' = \frac{1}{2m} (\hat{\mathbf{p}} - q\mathbf{A}')^2 + q\phi' \quad (62)$$

but the basic physics is unchanged as one can show that the solutions are related by a simple phase factor, namely

$$\psi'(\mathbf{r}, t) = \psi(\mathbf{r}, t)e^{i\Lambda(\mathbf{r}, t)} \quad (63)$$

where

$$\Lambda(\mathbf{r}, t) = \frac{q}{\hbar} f(\mathbf{r}, t) \quad (64)$$

The constant force problem we have considered can be considered as a case of a uniform field in the specific gauge configuration given by

$$\text{first gauge:} \quad \phi = -Ex \quad \mathbf{A} = 0 \quad (65)$$

A constant electric field is also obtained from Eqns. 58 via the scalar and vector potentials

$$\text{second gauge:} \quad \phi' = 0 \quad \mathbf{A} = -\hat{i}Et \quad (66)$$

The gauge function connecting the two cases is $f(\mathbf{r}, t) = -Ext$, so that solutions of the Schrödinger equation in the two gauges should be related via

$$\psi'(\mathbf{r}, t) = e^{iq(-Ext)/\hbar} \psi(\mathbf{r}, t) = e^{-iFxt/\hbar} \psi(\mathbf{r}, t) \quad (67)$$

In the first gauge, wavepacket solutions for a constant force can be obtained from any initial state via the time-development operator in Eqn. 50 since

$$\hat{H}_F = \frac{p^2}{2m} - Fx \quad (68)$$

where $F = qE$ and we use

$$\psi(x, t) = e^{-i\hat{H}_F t/\hbar} \psi(x, 0) \quad (69)$$

The Hamiltonian related to this in the second gauge is

$$\hat{H}' = \frac{1}{2m} (\hat{p} - q(-Et))^2 = \frac{\hat{p}^2}{2m} + \frac{Ft\hat{p}}{m} + \frac{F^2t^2}{2m} \quad (70)$$

so that the solutions, $\psi'(x, t)$ must satisfy

$$\hat{H}'\psi'(x, t) = i\hbar \frac{\partial}{\partial t} \psi'(x, t) \quad (71)$$

In this case, the Hamiltonian is not formally time-independent and we must generalize Eqn. 2 by integrating with respect to t . The formal solution can then be written in the form

$$\begin{aligned} \psi'(x, t) &= \exp \left[-\frac{i}{\hbar} \left(\frac{\hat{p}^2 t}{2m} + \frac{Ft^2 \hat{p}}{2m} + \frac{F^2 t^3}{6m} \right) \right] \psi'(x, 0) \\ &= e^{-iFtx/\hbar} \left[e^{-i\hat{H}_F t/\hbar} \psi(x, 0) \right] \end{aligned} \quad (72)$$

$$= e^{-iFtx/\hbar} \psi(x, t) \quad (73)$$

The phase change on gauge transformation is seen to arise in a very explicit way for any $\psi(x, t)$, not just for the Gaussian initial state.

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Appendix

Because the quantum mechanical problem of a particle subject to a constant force is often handled using propagator methods, we very briefly review the relevant results here. The propagator in momentum space can be written in the form

$$K(p, p'; t, 0) = \sum_E \phi_E^*(p') \phi_E(p) e^{-iEt/\hbar} \quad (74)$$

where ϕ_E are the energy eigenstates of the appropriate Schrödinger equation in momentum space. The time development of the wavefunction is then given by

$$\phi(p, t) = \int_{-\infty}^{+\infty} K(p, p'; t, 0) \phi(p', 0) dp' \quad (75)$$

The energy eigenstates corresponding to the uniformly accelerated particle described by Eqn. 25 are

$$\phi_E(p) = C e^{i(Ep - p^3/6m)/\hbar F} \quad (76)$$

where the normalization constant is given by $C = 1/\sqrt{2\pi\hbar F}$ if the $\phi_E(p)$ are normalized via

$$\int_{-\infty}^{+\infty} \phi_E^*(p) \phi_{E'}(p) dp = \delta(E - E') \quad (77)$$

Using Eqn. 76, the propagator is given by

$$\begin{aligned} K(p, p'; t, 0) &= \int dE \phi_E^*(p') \phi_E(p) e^{-iEt/\hbar} \\ &= e^{(p'^3 - p^3)/6m\hbar F} \left[\frac{1}{2\pi\hbar F} \int_{-\infty}^{+\infty} dE e^{iE(p - p' - Ft)/\hbar F} \right] \\ &= e^{(p'^3 - p^3)/6m\hbar F} \delta(p - p' - Ft) \end{aligned} \quad (78)$$

The general time-dependent momentum-space solution is given in terms of the initial state $\phi(p', 0) = \phi_0(p')$ via Eqn. 75 as

$$\phi(p, t) = \phi_0(p - Ft) e^{i((p - Ft)^3 - p^3)/6m\hbar F} \quad (79)$$

in agreement with Eqn. 30.

The propagator in position space is defined similarly to Eqn. 74 and can be written in terms of Fourier transforms as follows:

$$\begin{aligned}
K(x, x'; t, 0) &= \sum_E \psi_E^*(x') \psi_E(x) e^{-iEt/\hbar} \\
&= \left(\frac{1}{\sqrt{2\pi\hbar}} \right)^2 \sum_E \int_{-\infty}^{+\infty} e^{-ix'p'/\hbar} dp' \int_{-\infty}^{+\infty} e^{ixp/\hbar} dp \phi_E^*(p') \phi_E(p) e^{-iEt/\hbar} \\
&= \left(\frac{1}{2\pi\hbar} \right) \int_{-\infty}^{+\infty} e^{-ix'p'/\hbar} dp' \int_{-\infty}^{+\infty} e^{ixp/\hbar} dp K(p, p'; t, 0)
\end{aligned} \tag{80}$$

which then gives the time-evolution of an initial $\psi(x, 0)$ via

$$\psi(x, t) = \int_{-\infty}^{+\infty} K(x, x'; t, 0) \psi(x', 0) \tag{81}$$

Using the result in Eqn. 78 and the Gaussian integral in Eqn. 10 we find that

$$K(x, x'; t, 0) = \sqrt{\frac{m}{2\pi i \hbar t}} e^{iFt(x' - Ft^2/6m)/\hbar} e^{im(x' - x - Ft^2/2m)^2/2\hbar t} \tag{82}$$

One can easily check that this form, when acting on a Gaussian initial state (as in Eqn. 19) gives the result in Eqn. 52.

One can also explicitly show that the expectation value of position using any initial state corresponds to uniformly accelerated motion by calculating

$$\begin{aligned}
\langle x \rangle_t &= \int_{-\infty}^{+\infty} \psi^*(x, t) x \psi(x, t) dx \\
&= \int_{-\infty}^{+\infty} dx x \int_{-\infty}^{+\infty} dx' K^*(x, x'; t, 0) \psi^*(x', 0) \int_{-\infty}^{+\infty} dx'' K(x, x''; t, 0) \psi(x'', 0)
\end{aligned} \tag{83}$$

The integral over x can be done first by using the result

$$\begin{aligned}
\int_{-\infty}^{+\infty} dx x K^*(x, x'; t, 0) K(x, x''; t, 0) &= \left(\frac{\hbar t}{im} \right) e^{im[(x'')^2 - (x')^2]/2\hbar t} e^{(im/\hbar t)(Ft^2/2m)(x' - x'')} \\
&\quad \times \frac{\partial}{\partial x''} [\delta(x' - x'')]
\end{aligned} \tag{84}$$

and then integrating by parts to move the derivative with respect to x'' to act on the other factors; the form in Eqn. 57 then follows immediately.

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