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# **New Journal of Physics**

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### A representation-free description of the Kasevich–Chu interferometer: a resolution of the redshift controversy

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New Journal of Physics **15** (2013) 013007 (48pp) Received 18 July 2012 Published 7 January 2013 Online at http://www.njp.org/ doi:10.1088/1367-2630/15/1/013007

**Abstract.** Motivated by a recent claim by Müller *et al* (2010 *Nature* **463** 926–9) that an atom interferometer can serve as an atom clock to measure the gravitational redshift with an unprecedented accuracy, we provide a representation-free description of the Kasevich-Chu interferometer based on operator algebra. We use this framework to show that the operator product determining the number of atoms at the exit ports of the interferometer is a *c*-number phase factor whose phase is the sum of only *two* phases: one is due to the acceleration of the phases of the laser pulses and the other one is due to the acceleration of the atom. This formulation brings out most clearly that this interferometer is an accelerometer or a gravimeter. Moreover, we point out that in different representations of quantum mechanics such as the position or the momentum representation the phase shift appears as though it originates from different physical phenomena. Due to this representation dependence conclusions concerning an enhanced accuracy derived in a specific representation are unfounded.

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#### 1. Introduction

The wave–particle dualism of quantum mechanics [1], with its mind boggling manifestations such as Einstein–Podolsky–Rosen correlations [2], delayed choice experiments [3] and the quantum eraser [4] to name a few, has always been and still is a conundrum; in recent years there has been a shift in the paradigm. Rather than trying to understand these alien features of quantum theory we put them to use for technological applications. Indeed, the new field of quantum technology has emerged giving birth to quantum cryptography and quantum information processing with the long term goal of a building quantum computer.

#### 1.1. At the interface of quantum mechanics and general relativity

At the same time, the wave nature of matter has opened a new avenue for precision testing of the foundations of physics. Indeed, matter wave interferometry has come a long way from the original experiment of scattering electrons from a single crystal of nickel by Davisson and Germer [5] via neutron interferometry [6] to electron [7], atom, or molecule interferometers [8]; even large molecules such as  $C_{60}$  show interference properties [9]. A new era has started with the creation of cold atomic beams and the use of light fields as beam splitters [10, 11] and ultra-cold atoms in the form of Bose–Einstein condensates. Here, new tests of general relativity [12], such as the gravito-magnetic field governing the Lense–Thirring effect [13–15], are now within reach by atom interferometry [16–18]. Since atoms experience gravity, such precision tests require microgravity as provided by the International Space Station, and there is indeed a new drive to put atom interferometers into space [19].

An important step toward this goal is a recent experiment performed at the drop tower in Bremen [20] where a Bose–Einstein condensate was created and measured while in free fall. Similarly, the experiments demonstrating interferometry with laser-cooled atoms on a parabolic flight of a plane [21–23] or with Bose–Einstein condensates at the drop tower [24] provide important stepping stones toward tests of general relativity [25] such as the equivalence principle with the wave nature of matter. In this context we also draw attention to the measurement of the quantized energy levels of a neutron in the gravitational field [26] and the recent application of the Ramsey method to measure the gravitationally induced shift [27, 28].

These experiments build on the extremely beautiful and seminal neutron-interference experiment [29–31] by Roberto Collela, Albert Overhauser, and Sam Werner (COW) which was carried out over 35 years ago and which for the first time saw a matter wave interference effect due to gravity. Even then the question arose whether one could see in such an arrangement relativistic effects and the question was largely resolved [32, 33].

However, recently in the context of atom optics [34, 35] similar questions came up again. Indeed, it has been claimed [36] that one can measure the gravitational redshift in the Kasevich–Chu atom interferometer [37] with a much greater precision than in other measurements schemes. This claim has been disputed [38, 39] in a series of papers, an exciting discussion [40–47] has emerged and new ideas [48–50] have been put forward.

#### 1.2. The redshift controversy

In the Kasevich–Chu atom interferometer [37] shown in figure 1, an atomic beam interacts with three short laser pulses which coherently split and recombine the beam. The number of atoms

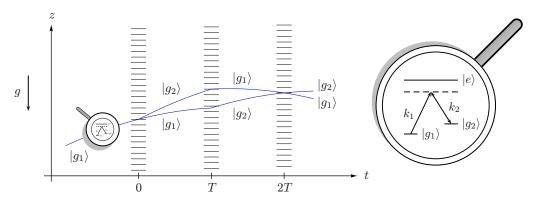


Figure 1. Kasevich—Chu atom interferometer represented in space—time. Three laser pulses at the times t = 0, T and 2T induce two-photon transitions in an atom between the ground state  $|g_1\rangle$  and the state  $|g_2\rangle$  through a virtual state which is detuned from the excited state  $|e\rangle$ . These transitions are accompanied by a momentum transfer  $\pm \hbar k$  where the plus or minus signs correspond to the transition from  $|g_1\rangle$  to  $|g_2\rangle$ , or from  $|g_2\rangle$  to  $|g_1\rangle$ , respectively. As a result the laser pulses coherently split and recombine the atomic beam moving against a linear gravitational potential aligned along the z-axis. With appropriately chosen parameters the laser pulses at the t = 0 and 2T act as beam splitters, whereas the one at t = T serves as a mirror. The two paths leading after the time 2T to an atom either being in the state  $|g_1\rangle$  or  $|g_2\rangle$  interfere and the counts of atoms in these two exit ports depend on the sum of two phases. (i) The difference  $\delta \phi \equiv \phi(2T) - 2\phi(T) + \phi(0) \cong \ddot{\phi}(0)T^2$  between the phases of the three laser pulses represents the discrete version of the second derivative  $\ddot{\phi}$  of  $\phi = \phi(t)$  in time. (ii) The phase  $\delta \varphi = k\ddot{z}T^2$  results from the quantum mechanical commutation relation between position and momentum. Hence, the total phase  $\alpha \equiv \delta \phi + \delta \varphi$  of the Kasevich–Chu interferometer is the sum of the accelerations of the laser phase and the atom which with  $\ddot{z} = -g$  reads  $\alpha = \delta \phi - \delta \varphi_g$  where  $\delta \varphi_g \equiv kg T^2$ . The classical trajectories which are bent due to the gravitational field are independent of the phases of the laser pulses. However, the de Broglie wave of the atom is sensitive to them and, the appearance of  $\delta \phi$  is a manifestation of the scalar Aharanov–Bohm effect. Moreover, the phase  $\delta \varphi_g$  is a consequence of the different time ordering on the two paths: on the upper one the atom travels in the gravitational field first with the momentum  $p + \hbar k$  and then with p whereas in the lower path it is the other way around.

in the two exit beams is determined by the difference in phase between the de Broglie waves on the two paths.

We emphasize that there is a great similarity between the Kasevich–Chu atom interferometer and the COW neutron interferometer. Therefore, one might wonder if one could not just transfer the results from one to the other. However, there are subtle differences between these two devices which shall be discussed elsewhere [51].

Today several approaches [52–55] to describe atom optics in gravitational fields, and to obtain this phase difference, exist. The approach [52] most relevant for the present discussion

is based on the Feynman path integral [56]. Here the phase of the wave function arises from the propagation along the classical trajectories and the interaction with the laser pulses. This technique is well suited for the connection [57] to general relativity since according to Louis de Broglie [58] the phase of a matter wave is proportional to the proper time which in the non-relativistic limit reduces to the Lagrangian integrated over the coordinate time [32, 33]. In this sense the appearance of the gravitational potential in the Lagrangian is a non-relativistic residue [59] of general relativity. It is this formalism that has been central to the controversy surrounding the redshift.

The Feynman path integral approach lives in space–time, that is, it is expressed in terms of the continuous spectrum of eigenvalues of the position operator and the coordinate time. Due to this choice of the quantum mechanical representation the physical origin of the phase shift in the interferometer is attributed to the interaction of the atom with the laser and not to its time evolution in the gravitational field between the pulses. However, the controversy about the redshift has originated from the division of terms in the semi-classical approach contributing to the phase shift in the interferometer into four parts: one from the kinetic and one from the potential energy in the Lagrangian, one due to the phases of the laser pulses and one from the interaction of the atom with the laser field. When the phases of the laser fields are timeindependent only three terms are relevant. They have the same magnitude but differ in their signs. Indeed, the phases due to the kinetic and the potential energy are positive whereas the one due to the laser interaction is negative. One can therefore interpret the phase in the interferometer as the result of the cancellation of the phases either due to the kinetic and potential energy, or due to the kinetic energy and the laser interaction. In the first case the phase of the interferometer is a consequence of the interaction of the atom with the laser. In the second interpretation it is due to the potential energy and therefore due to the redshift. Hence, the cancellation of these terms is crucial for the argument.

In the present paper we demonstrate that this decomposition of phases and their interpretation in terms of physical phenomena actually depends on the specific quantum mechanical representation chosen to perform the calculation. In order to bring out this fact most clearly we pursue an approach [60] based on operator algebra. In particular, we show that the phase of the interferometer is a consequence of a product of unitary time evolution operators which with the help of the canonical commutation relations between position and momentum operators reduce to a single c-number phase factor. Therefore, when we evaluate this product in a particular representation, either position, or momentum, or energy, we of course always arrive at the same c-number phase factor.

However, the way in which this term arises will depend crucially on the chosen representation. In the position representation which is at the very heart of the Feynman path integral approach the phase shift in the interferometer emerges from a cancellation of terms which is completely different when we employ the momentum representation. Therefore, it is dangerous to derive conclusions about improved accuracy from the cancellation of terms in one specific representation as it was done in [36]. Moreover, our operator approach shows that the phase in this interferometer is the difference of the accelerations of the laser phase and the atom in the gravitational field. This feature allows us to analyze the interferometer in different scenarios which brings out the different roles of these phases.

This representation dependence is reminiscent of calculating a quantum mechanical expectation value by employing quantum mechanical phase space distribution functions [61]. Indeed, there exist many such phase space functions and they all take on different values in

phase space. Nevertheless, each of them is associated with a specific operator ordering such that expectation values of so-ordered operators with the corresponding phase space distribution functions yield the correct quantum mechanical results. However, no specific operator ordering is above another.

#### 1.3. Outline of article

Our article which is the more detailed companion of a shorter version [62] is organized as follows: we start in section 2 by reviewing the connection between the phase of a de Broglie wave, proper time in general relativity and the non-relativistic Lagrangian. In section 3 we briefly summarize the essential ingredients of the Kasevich–Chu atom interferometer and then provide a semiclassical description of it based on the result of section 2 that the phase of a matter wave is given by the classical action. We devote section 4 to our operator algebra approach toward the interferometer. We then in section 5 show the interplay between the two phases due to the accelerations of the phase and the atom discussing three scenarios. Sections 6 and 7 are dedicated to the demonstration of the representation-dependent interpretation of the contributing terms leading to the total phase shift in the interferometer. In section 8 we summarize our main results and provide an outlook.

In order to keep the paper self-contained we have included detailed calculations and derivations in several appendices. For example, we dedicate appendix A to a derivation of the effective Hamiltonian describing the interaction of a three-level atom with two short counterpropagating laser pulses which are far-detuned from the excited state. In particular, we show that this arrangement serves as a beam splitter or a mirror for atoms provided the parameters of the pulse are chosen appropriately. In appendix B we expand on the semi-classical approach toward the interferometer and provide a connection with the Wentzel–Kramers–Brillouin (WKB)-wave function. Moreover we resolve a small puzzle put forward in [60]. In appendix C we then recall an operator identity crucial for our study of the interferometer. We analyze in appendix D the time evolution of a momentum eigenstate in a linear potential and show that the state changes its eigenvalue according to Newtonian mechanics and accumulates the phase. Finally, in appendix E we present an alternative evaluation of the relevant matrix element in position space using the method of stationary phase.

#### 2. Non-relativistic residues

In the present section we briefly recall the fact that the classical action determining the phase of a matter wave is a non-relativistic residue of the proper time, that is of a relativistic origin.

In 1924 Louis de Broglie [58] published his far-reaching proposal of the existence of matter waves. It is interesting to note that the starting point of his considerations was the question of the transformation properties of energy and proper time under Lorentz transformations. In this way he arrived at the conclusion that the phase  $\beta_g$  of the matter wave  $\psi \equiv \exp(-i\beta_g)$  is given by

$$\beta_g \equiv \frac{mc^2}{\hbar} \tau,\tag{1}$$

where  $\tau$  is the proper time of the particle of rest mass m, and c and  $\hbar$  denote the speed of light and Planck's constant, respectively.

In general relativity  $\tau$  is determined by the space–time [25] parameterized by the Cartesian coordinates  $x^{\mu} \equiv (ct, x, y, z)$  with  $\mu = 0, 1, 2$  and 3 and characterized by the metric coefficients  $g_{\mu\nu}$  through the line element

$$c^{2} d\tau^{2} = ds^{2} = g_{\mu\nu} dx^{\mu} dx^{\nu}.$$
 (2)

In the limit of a weak gravitational field and a velocity

$$v^{(i)} \equiv \frac{\mathrm{d}x^{(i)}}{\mathrm{d}t} \equiv \dot{x}^{(i)},\tag{3}$$

which is small compared to c the metric coefficients reduce to

$$g_{00} \cong 1 + \frac{2}{c^2} \Phi, \quad g_{jj} \cong -1 \quad \text{and} \quad g_{ij} = 0$$
 (4)

for  $i \neq j$ .

Here and throughout the article dots indicate derivatives with respect to coordinate time t and  $\Phi = \Phi(\mathbf{r})$  is the Newtonian potential.

Hence, in the non-relativistic limit the proper time follows from the relation

$$d\tau \cong \left[1 - \frac{2}{c^2} \left(\frac{1}{2} \mathbf{v}^2 - \Phi\right)\right]^{1/2} dt \cong dt - \frac{1}{mc^2} \tilde{\mathcal{L}}_g dt, \tag{5}$$

where in the last step have expanded the square root and have introduced the non-relativistic Lagrangian

$$\tilde{\mathcal{L}}_g \equiv \frac{1}{2} m \mathbf{v}^2 - m \,\Phi. \tag{6}$$

As a result, the de Broglie wave  $\psi$  takes the form

$$\psi = e^{-i\beta_g} \cong \exp\left[-\frac{i}{\hbar}mc^2t\right] \exp\left[\frac{i}{\hbar}\int dt \,\tilde{\mathcal{L}}_g\right]$$
 (7)

and the appearance of  $\tilde{\mathcal{L}}_g$  and, in particular, of the kinetic and the potential energies in the phase  $\beta_g$  of the de Broglie wave is a consequence of the proper time. In this sense these energies are the non-relativistic residues of the proper time.

Indeed, the kinetic energy arises from the combination of the expansion of the relativistic square root containing the term  $(\mathbf{v}/c)^2$  and reflecting the phenomenon of time dilation in special relativity, and the multiplication by the factor  $mc^2$ . For this reason Müller *et al* [36] refer to the kinetic energy term as the time dilation term. Likewise, since the contribution due to the Newtonian gravitational potential  $\Phi$  gives rise to the redshift, Müller *et al* [36] call it the redshift term.

Although we support the notion of  $\tilde{\mathcal{L}}_g$  being the non-relativistic residue of the relativistic phase, we throughout this article adhere to the standard notation of kinetic and potential energy. Moreover, we emphasize that the potential energy only contains the gravitational interaction and not the interaction of the particle with an electromagnetic field. This fact will become important when we discuss in the next section the Kasevich–Chu interferometer.

We conclude this section by noting that the first contribution in (7) results from the rest mass of the atom. In an interferometer with two paths of identical coordinate time *t* the resulting phase shifts from this term are therefore identical, and not of interest in the standard Kasevich–Chu interferometer. However, there might be situations where it will be important [49] but they are not analyzed in the present article.

#### 3. Kasevich-Chu atom interferometer: classical and semi-classical considerations

In order to keep the article self-contained we first briefly review the essential ingredients of the Kasevich-Chu atom interferometer used in [37] and shown in figure 1. We then analyze the classical trajectories of an atom moving under the influence of gravity and three short laser pulses. The idea that the phase shift in the interferometer is governed by the corresponding action motivates our study of the dynamical phases corresponding to the kinetic and gravitational potential energies as well as the interaction with the laser pulses along the closed classical path of the atom in the interferometer. We show that they are closely connected which allows us to combine the terms contributing to the total phase shift in several different ways and to attribute its origin to different physical phenomena.

#### 3.1. The inner workings of the interferometer

For the sake of clarity we consider a one-dimensional motion of the atom along the z-axis. The constant gravitational field of acceleration g points in the negative z-direction. Initially the atom is in its ground state  $|g_1\rangle$ .

At time t=0 a short laser pulse excites via a two-photon transition the atom into a superposition of the states  $|g_1\rangle$  and  $|g_2\rangle$ . The parameters of the pulse, such as the pulse length and its electric field strength are adjusted as to create a superposition of  $|g_1\rangle$  and  $|g_2\rangle$  with equal weights. As discussed in the next subsection this transition is accompanied by a momentum transfer of  $\hbar k$  where k is the wave vector of the sum of the wave vectors of the two photons. This process leads to a coherent splitting of the atomic beam into an upper and a lower path. Throughout our article we assume that the pulse is so short that the atom does not move during its duration.

At time T a second pulse interacts with the atom. As a result the atom on the upper path moving in  $|g_2\rangle$  goes into the ground state  $|g_1\rangle$  and the momentum is reduced by  $\hbar k$ . In contrast, the atom on the lower path moving in the ground state  $|g_1\rangle$  makes a transition to  $|g_2\rangle$  and increases its momentum by  $\hbar k$ . This pulse is adjusted so that the atom makes the transitions with absolute certainty.

At time t=2T a third laser pulse interacts with the atom and the two paths recombine. For this purpose the parameters of the pulse are chosen in such a way as to create again a superposition with equal weights. As a result the atom in the state  $|g_1\rangle$  in the upper path can either go to  $|g_2\rangle$  and increase its momentum by  $\hbar k$  leaving the set-up in the excited state  $|g_2\rangle$ , or continue in  $|g_1\rangle$  with the same momentum. The atom in the lower path in  $|g_2\rangle$  has also two alternatives: it can continue in  $|g_2\rangle$  or reduce its momentum by  $\hbar k$  and arrive in  $|g_1\rangle$ . Hence, for each of the two exits there exist two paths that lead to them.

#### 3.2. Classical trajectories

We now evaluate the classical trajectories resulting from the Euler–Lagrange equations

$$\frac{\mathrm{d}}{\mathrm{d}t}\frac{\partial \mathcal{L}}{\partial \dot{z}} - \frac{\partial \mathcal{L}}{\partial z} = 0,\tag{8}$$

where the Lagrangian

$$\mathcal{L} \equiv \frac{1}{2}mv^2 - V_g(z) - V_{lp}(z, t) \tag{9}$$

involves, apart from the kinetic energy with the velocity  $v \equiv \dot{z}$ , also the linear potential

$$V_g(z) \equiv mgz \tag{10}$$

due to the constant gravitational field, and the space- and time-dependent potential

$$V_{\rm lp}(z,t) \equiv \sum_{j=0}^{2} \delta(t-jT)J_{j}(z) \tag{11}$$

created by the three laser pulses at the times t = 0, T and 2T.

As shown in appendix A the potential  $V_{lp}$  describes the beam splitters and mirrors for the atoms, and the actions

$$J_{j}(z) \equiv \begin{cases} -\hbar[kz + \phi(jT)] \\ +\hbar[kz + \phi(jT)] \\ 0 \end{cases}$$
(12)

correspond to transitions from  $|g_1\rangle$  to  $|g_2\rangle$  and  $|g_2\rangle$  to  $|g_1\rangle$  indicated by the minus and the plus sign, respectively, or no interaction at time t=jT.

When we substitute the Lagrangian (9) into the Euler-Lagrange equations (8) we find with the help of the explicit forms (10)–(12) of the potentials the classical equation of motion

$$\dot{p}(t) = -mg + \sum_{j=0}^{2} \delta(t - jT)p_{j}, \tag{13}$$

for the momentum  $p(t) \equiv mv(t) \equiv m\dot{z}(t)$  where the momentum transfer

$$p_{j} \equiv \begin{cases} +\hbar k \\ -\hbar k \\ 0 \end{cases} \tag{14}$$

in the jth laser pulse results from the transitions  $|g_1\rangle$  to  $|g_2\rangle$  and from  $|g_2\rangle$  to  $|g_1\rangle$ , respectively, or from no interaction.

Integration of (13) yields

$$p(t) = p_g(0) - mgt + \sum_{j=0}^{2} \Theta(t - jT)p_j \equiv p_g(t) + \sum_{j=0}^{2} \Theta(t - jT)p_j.$$
 (15)

Here  $p_g(0)$  and  $\Theta$  are the momentum of the atom shortly before the first laser pulse and the Heaviside step function, respectively.

The transition from  $|g_1\rangle$  to  $|g_2\rangle$  at the times t=jT of the laser pulses increases the momentum  $p_g(jT) \equiv p_g(0) - mgjT$  of the atom due to the gravitational field by  $\hbar k$ , whereas the transition from  $|g_2\rangle$  to  $|g_1\rangle$  decreases it by  $\hbar k$ . In case of no interaction the momentum transfer  $p_j$  vanishes. We emphasize that the phase  $\phi = \phi(jT)$  of the pulse does not enter into the Newtonian dynamics of the atom since  $\phi$  is only time but not space dependent.

When we integrate the equation of motion

$$v(t) \equiv \dot{z}(t) = v_g(0) - gt + \sum_{j=0}^{2} \Theta(t - jT) \frac{p_j}{m}$$
 (16)

for the velocity following from (15) with  $v_g(0) \equiv p_g(0)/m$  we find the trajectory

$$z(t) = z_g(t) + \sum_{j=0}^{2} \int_{-\infty}^{t} dt' \,\Theta(t' - jT) \frac{p_j}{m}.$$
 (17)

Here

$$z_g(t) \equiv z_g(0) + v_g(0)t - \frac{1}{2}gt^2$$
(18)

describes the motion solely in the linear gravitational potential and  $z_g(0)$  is the position of the atom just before the first laser pulse. Throughout the article we adhere to a notation where we denote trajectories following from the Lagrangian  $\mathcal{L}$  given by (9) and including the gravitational potential as well as the laser pulses by z = z(t) and v = v(t). In contrast, we call the trajectories associated with the Lagrangian

$$\mathcal{L}_g \equiv \frac{1}{2}mv^2 - V_g(z) \tag{19}$$

in the presence of gravity but the absence of the pulses by  $z_g = z_g(t)$  and  $v_g = v_g(t)$ .

In table 1 we compile the time-dependent coordinates and velocities of the atom in the two arms of the interferometer.

#### 3.3. Phase shift from action

In section 2 we have shown that the phase of a de Broglie wave is the action in units of  $\hbar$ . However, this derivation has relied on the fact that the only interaction of the atom is of a gravitational nature. In the case of the atom interferometer we have in addition the interaction with laser pulses. We assume that the phase shift  $\alpha$  is still given by the action

$$\alpha = \frac{1}{\hbar} \oint dt \, \mathcal{L} \tag{20}$$

of the complete Lagrangian  $\mathcal{L}$  evaluated along the closed classical trajectory of the atom in the interferometer following from the Euler-Lagrange equations (8). Here we always subtract the contributions originating from the lower path from the ones of the upper path.

We emphasize that (20) is an extrapolation of (7) that is frequently made. In particular, all articles [36–52] relevant for the redshift controversy start from this assumption. Moreover, we recall that the cancellation of terms which serves as the theoretical underpinning of the claims made in [36] is based on (20). It is for this reason that we now briefly discuss the consequences of (20). Moreover, these considerations also lay the ground work for section 7 where we compare and contrast the exact quantum calculation in position space with this semi-classical result, and in particular, with the way the total phase shift  $\alpha$  arises in the exact and in the semi-classical approach. In section 7 we show that these actions do not appear in the exact analysis.

In appendix B we compare and contrast the Lagrange approach toward quantum mechanics to the more familiar Hamilton one in the semi-classical limit. We show that in the case of an energy wave function the phase  $\alpha$  given by (20) leads us to the well-known phase of a WKB-wave. Since this treatment is independent of the assumption that the interaction originates from gravity the expression for  $\alpha$  provides a convincing argument the  $\alpha$  is correct even for a particle in the presence of non-gravitational fields.

**Table 1.** Evaluation of the dynamical phases corresponding to the kinetic and potential energy along the closed path of the interferometer. Here we always subtract the contributions arising from the lower path from the ones occurring on the upper path. In the two columns we display the Newtonian dynamics between the first and the second, and between the second and third laser pulse, respectively. The time variable covers the complete domain  $0 \le t \le 2T$ . Moreover, we have introduced for the sake of clarity the abbreviations  $v_g(t) \equiv v_g(0) - gt$  and  $z_g(t) \equiv z_g(0) + v_g(0)t - gt^2/2$  for the velocity and position of the atom in the gravitational field.

	Between $0$ and $T$	Between $T$ and $2T$	
Velocity $v_{\rm u}$ on upper path	$v_g(t) + \frac{\hbar k}{m}$	$v_g(t)$	
Velocity $v_1$ on lower path	$v_g(t)$	$v_g(t) + \frac{\hbar k}{m}$	
Difference $v \equiv v_{\rm u} - v_{\rm l}$ in velocities	$\frac{\hbar k}{m}$	$-\frac{\hbar k}{m}$	
Sum $v_+ \equiv v_u + v_l$ of velocities	$2v_g(t) + \frac{\hbar k}{m}$	$2v_g(t) + \frac{\hbar k}{m}$	
Action due to kinetic energy			
$\int_0^{2T} dt  \frac{1}{2} m (v_u^2 - v_l^2)$ $= \frac{1}{2} m \int_0^{2T} dt  v_+ v$	$\hbar k \int_0^T \! \mathrm{d}t  \left[ v_g(t) + \frac{\hbar k}{2m} \right]$	$-\hbar k \int_T^{2T} dt \left[ v_g(t) + \frac{\hbar k}{2m} \right]$	
Dynamical phase due to kinetic energy $\frac{1}{\hbar} \oint dt  \frac{1}{2} m v^2$	$-k[z_g(2T) - 2z_g(T) + z_g(0)] = -k\ddot{z}_g(0)T^2 = kgT^2 = \delta\varphi_g$		
Upper path z <sub>u</sub>	$z_g(t) + \frac{\hbar k}{m}t$	$z_g(t) + \frac{\hbar k}{m} T$	
Lower path $z_1$	$z_g(t)$	$z_g(t) + \frac{\hbar k}{m} \left( t - T \right)$	
Difference $z_{-} \equiv z_{\rm u} - z_{\rm l}$	$\frac{\hbar k}{m} t$	$\frac{\hbar k}{m} \left( 2T - t \right)$	
$\int_0^{2T} \mathrm{d}t \ mg \ z$	$\hbar kg \int_0^T \! \mathrm{d}t \ t$	$\hbar kg \int_T^{2T} \! \mathrm{d}t  (2T - t)$	
Dynamical phase due to gravitational energy $\frac{1}{\hbar} \oint dt \ mg \ z$	$k g T^2 \equiv$	$\delta arphi_g$	

#### 3.4. Actions of kinetic and potential energies and laser pulses

We start our analysis of the semi-classical phase shift  $\alpha$  following from (20) by evaluating the action associated with the complete Lagrangian  $\mathcal{L}$ . Indeed, with the help of the expression (9) for  $\mathcal{L}$  we find

$$\oint dt \, \mathcal{L} = \oint dt \, \frac{1}{2} m v^2 - \oint dt \, V_g - \oint dt \, V_{lp}. \tag{21}$$

Next we calculate the actions associated with these three energies. In table 1 we establish the identity

$$\frac{1}{\hbar} \oint dt \, \frac{1}{2} m v^2 = \frac{1}{\hbar} \oint dt \, mgz = \delta \varphi_g \tag{22}$$

for the actions expressed in units of  $\hbar$  corresponding to the kinetic and gravitational energies on the closed classical path of the atom through the interferometer with the abbreviation

$$\delta\varphi_g \equiv kgT^2. \tag{23}$$

We now turn to the action due to the laser pulses. With the help of the delta function in  $V_{lp}$  defined by (11) we can immediately perform the integration over time and find combinations of the phases  $\mp [kz(jT) + \phi(jT)]$  with j=0, 1 and 2 at the times of the pulses. According to (12) the minus and plus signs correspond to the transitions  $|g_1\rangle$  to  $|g_2\rangle$  and  $|g_2\rangle$  to  $|g_1\rangle$ , respectively. Moreover, we have to take into account that at T the position  $z_u(T)$  of the atom on the upper arm is different from the one on the lower arm which we denote by  $z_1(T)$ . Needless to say, we assume start and end points z(0) and z(2T) to be identical in the two arms. We shall show in section 7 that this assumption of the semi-classical approach follows in a strict sense from the exact quantum mechanical calculation of position space.

As a result we arrive at the expression

$$\frac{1}{\hbar} \oint dt \ V_{lp} = -\left\{ \left[ kz(2T) + \phi(2T) \right] - \left[ kz_{l}(T) + \phi(T) \right] \right\} + \left[ kz_{u}(T) + \phi(T) \right] - \left[ kz(0) + \phi(0) \right]. \tag{24}$$

In quantum mechanics it is customary that an operator at an earlier time stands to the right of an operator at a later time. In (24) and throughout the article we adhere to this rule even when we deal with c-numbers since it brings out most clearly how the individual contributions arise in the time evolution of the atom through the interferometer. Indeed, on the upper path we go from  $|g_1\rangle$  to  $|g_2\rangle$  at t=0 which introduces a minus sign in front of the last square bracket and return at T to  $|g_1\rangle$ . This process is associated with a plus sign. On the lower arm the same sequence is shifted in time by T, that is we reach  $|g_2\rangle$  at T and return to  $|g_1\rangle$  at 2T. Moreover, we subtract the contributions from the lower path from the upper path.

When we combine the terms we arrive at

$$\frac{1}{\hbar} \oint dt \ V_{lp} = -[\delta \phi + \delta \varphi], \tag{25}$$

where we have introduced the difference

$$\delta\phi \equiv \phi(2T) - 2\phi(T) + \phi(0) \tag{26}$$

between the phases of the laser pulses at the three interactions times, and the phase

$$\delta \varphi \equiv k \delta z = k[z(2T) - z_1(T) - z_0(T) + z(0)] \tag{27}$$

due to the positions of the atom at the times of the laser pulses.

It is interesting to note that the phase  $\delta \phi$  is the discrete version of the second derivative of the phase with respect to time. For a quadratic variation of  $\phi$  in time this result is even exact. Hence, one contribution to the dynamical phase associated with the laser pulse arises from the acceleration of the phase of the pulses. The other contribution emerges from a combination of coordinates of the atom which is again reminiscent of a second derivative. However,  $\delta \varphi$  contains the sum  $z_u(T) + z_1(T)$  of the positions of the atom in the two arms rather than 2z(T).

Nevertheless, we recover the acceleration when we recall from the bottom part of table 1 the relation

$$\delta z = \left[ z_g(2T) + \frac{\hbar k}{m} T \right] - z_g(T) - \left[ z_g(T) + \frac{\hbar k}{m} T \right] + z_g(0), \tag{28}$$

that is

$$\delta z = z_{\varrho}(2T) - 2z_{\varrho}(T) + z_{\varrho}(0) \tag{29}$$

which demonstrates that in  $\delta z$  only  $z_g$  appears. Moreover, it enters in the form of a second derivative in time and therefore brings in the acceleration  $\ddot{z}_g$  of the atom due to gravity. One might suspect that the appearance of the acceleration of the atom is limited to the case of a linear potential. However, in the representation-free description of the interferometer based on operator algebra we show that due to the different sequence of events in the two arms the commutation relations of quantum mechanics lead to the acceleration even for a potential of arbitrary shape.

When we now substitute the expression (29) for  $\delta z$  into the formula (27) for  $\delta \varphi$  we find

$$\delta \varphi = k \ddot{z}_g T^2 = -kg T^2 = -\delta \varphi_g, \tag{30}$$

and the accumulated phase due to the interaction with the laser pulses reads

$$\frac{1}{\hbar} \oint dt \ V_{lp} = -[\delta \phi - \delta \varphi_g]. \tag{31}$$

We emphasize that the phase  $\phi$  of the laser pulse enters in a rather decisive way. Although  $\phi$  does not contribute to the classical trajectories it appears in the quantum mechanical description as a phase. In this sense the appearance of  $\phi$  is a manifestation of the scalar Aharanov–Bohm effect.

We conclude by noting that the relation

$$\frac{1}{\hbar} \oint dt \, \frac{1}{2} m v^2 - \frac{1}{\hbar} \oint dt \, mgz = \delta \varphi_g - \delta \varphi_g = 0 \tag{32}$$

following from equation (22) suggests the identity

$$\oint dt \, \mathcal{L}_g = 0, \tag{33}$$

where  $\mathcal{L}_g$  is the Lagrangian (19) describing the motion of the atom solely due to the gravitational field. However, such an interpretation is misleading since the identity (22) of the actions due to kinetic and gravitational energy is a result of the full Lagrangian  $\mathcal{L}$  given by (9) which also includes the potential  $V_{lp}$  created by the laser pulses and acting as the beam splitters and mirrors of the interferometer. Indeed, for the identity (22) we need the two distinct arms of the interferometer which are a result of the interactions of the atom with the laser pulses, and therefore of  $V_{lp}$ . Needless to say, the trajectories following solely from  $\mathcal{L}_g$  do not provide two but only a single path connecting two points in space during the time 2T. Nevertheless, the identity (22) still holds true but on a rather trivial level since in this case both actions vanish identically. This property is in full accordance with the fact that  $\delta \varphi_g$  vanishes for k = 0, that is in the absence of a momentum transfer.

#### 3.5. Different orderings yield different interpretations of phase shift

We are now in a position to calculate the total phase shift  $\alpha$  in the interferometer. From equation (21) we note that  $\alpha$  is given by the sum of three terms. Since we are in the semi-classical limit these contributions are c-numbers rather than operators. As a result we can combine them in several different ways and each combination is connected with a different interpretation.

For example, we may consider the order

$$\oint dt \, \mathcal{L} = \left[ \oint dt \, \frac{1}{2} m v^2 - \oint dt \, V_g \right] - \oint dt \, V_{lp}. \tag{34}$$

Due to the identity (22) the first two terms cancel each other and with the help of (25) we arrive at

$$\alpha = \frac{1}{\hbar} \oint dt \, \mathcal{L} = -\frac{1}{\hbar} \oint dt \, V_{lp} = \delta \phi - \delta \varphi_g. \tag{35}$$

Hence, this analysis suggests that  $\alpha$  arises solely from the interaction of the atom with the laser pulses, a point which has been stressed repeatedly in [38, 39, 52].

In contrast, Müller et al [36] have proposed to combine the terms in the way

$$\oint dt \, \mathcal{L} = \left[ \oint dt \, \frac{1}{2} m v^2 - \oint dt \, V_{lp} \right] - \oint dt \, V_g, \tag{36}$$

which due to (22) and (31) leads us to

$$\alpha = \frac{1}{\hbar} \oint dt \, \mathcal{L} = \left[ \delta \varphi_g + (\delta \phi - \delta \varphi_g) \right] - \oint dt \, V_g = \delta \phi - \delta \varphi_g, \tag{37}$$

in full agreement with (35). However, now the interpretation of the origin of the phase shift  $\alpha$  is completely different from the first choice of order. Indeed, we have obtained a mixed representation in which the  $\alpha$  arises partly from the interaction with the laser giving rise to  $\delta \phi$ , and partly from the action due to the gravitational potential producing  $-\delta \varphi_g$ . It is this interpretation of the cancellation of terms which is at the very heart of the redshift controversy. However, as shown in sections 6 and 7 the three phase terms in (21) do not occur in the momentum nor in the position representation of the exact quantum mechanical calculation.

#### 3.6. A perturbative treatment of the gravitational phase shift

The lower part of table 1 illustrates that the influence of the gravitational field cancels out in the difference

$$z_{-}(t) \equiv z_{\mathrm{u}}(t) - z_{\mathrm{l}}(t) = \begin{cases} \frac{\hbar k}{m} t & \text{for } 0 \leqslant t < T, \\ \frac{\hbar k}{m} (2T - t) & \text{for } T \leqslant t \leqslant 2T, \end{cases}$$

$$(38)$$

in height of the upper and lower path and is solely given by the momentum difference  $\hbar k$  between these trajectories. Therefore, we also arrive at the identity

$$\frac{1}{\hbar} \oint dt \ V_g = \frac{1}{\hbar} \oint dt \ mgz = \delta \varphi_g \tag{39}$$

if we evaluate the action associated with  $V_g$  not using the *exact* trajectories given by the Lagrangian  $\mathcal{L}$  but by the ones following from the Lagrangian

$$\mathcal{L}_f \equiv \frac{1}{2}mv^2 - V_{\rm lp},\tag{40}$$

consisting solely of the kinetic energy and the laser interaction. We emphasize that this approach is not consistent with the fact that we use the full Lagrangian  $\mathcal{L}$  to specify the phase shift but for the evaluation of the trajectories only  $\mathcal{L}_f$ . Nevertheless it still provides the correct answer since  $z_-$  given by (38) is independent of g.

#### 4. Phase shift as a consequence of time ordering: acceleration of atom

The states  $|\psi_1\rangle$  and  $|\psi_2\rangle$  of the center-of-mass motion in the two exit ports leading to  $|g_1\rangle$  and  $|g_2\rangle$ , respectively are a result of a sequence of unitary operations  $\hat{U}_g$ , or  $\hat{U}^{(\pm)}(t)$  on the initial state  $|\psi_i\rangle$  which reflect either the quantum mechanical motion of the atom in the gravitational field, or the interaction a laser pulse at time t, respectively. The plus or the minus sign in  $U^{(\pm)}$  correspond to the momentum change by  $\pm \hbar k$  due to the transitions from  $|g_1\rangle$  to  $|g_2\rangle$  or from  $|g_2\rangle$  to  $|g_1\rangle$ . We now analyze these products of unitary operators and rederive the phase shift in the interferometer using operator algebra.

#### 4.1. Sequence of events, probability and operator product

We emphasize that the order of events on the upper path is different from the one on the lower path. Indeed, pursuing the upper path leading to  $|g_1\rangle$  we first have transition to  $|g_2\rangle$ , followed by the motion in the gravitational field, return to  $|g_1\rangle$ , and again motion in the gravitational field. At the third pulse there is no interaction. Hence, on the upper path the sequence  $\hat{U}_u$  of unitary transformations reads

$$\hat{U}_{u} \equiv \hat{U}_{g} \; \hat{U}^{(-)}(T) \; \hat{U}_{g} \; \hat{U}^{(+)}(0). \tag{41}$$

In contrast, on the lower path also leading to  $|g_1\rangle$  the atom does not interact with the first laser pulse and remains in  $|g_1\rangle$ . As a result, we first have motion in the gravitational field, then a transition to  $|g_2\rangle$  due to the second laser pulse to be followed by motion in the gravitational field and finally return to  $|g_1\rangle$  due to the third laser pulse. Therefore, on the lower path the sequence  $\hat{U}_1$  of unitary transformations reads

$$\hat{U}_1 \equiv \hat{U}^{(-)}(2T) \; \hat{U}_g \; \hat{U}^{(+)}(T) \; \hat{U}_g. \tag{42}$$

The quantum state  $|\psi_1\rangle$  of the motion at the exit port for atoms in the ground state  $|g_1\rangle$  is the sum

$$|\psi_1\rangle = \frac{(-i)^2}{2}(\hat{U}_u + \hat{U}_1)|\psi_i\rangle$$
 (43)

of the evolutions along the two paths. As shown in appendix A the factor 1/2 arises from the two 50:50 beam splitters represented by the first and the third laser pulse and the factor  $(-i)^2$  reflects the two momentum kicks by the pulses.

As a result, the probability

$$P_{1} = \frac{1}{2} \left[ 1 + \frac{1}{2} (\langle \psi_{i} | \hat{U}_{1}^{\dagger} \hat{U}_{u} | \psi_{i} \rangle + \text{c.c.}) \right]$$
 (44)

to find the atom in the state  $|g_1\rangle$  at the exit of the interferometer is determined by the expectation value  $e \equiv \langle \psi_i | \hat{U}_1^\dagger U_u | \psi_i \rangle$  of the operator product  $\hat{U}_1^\dagger U_u$  in the initial state  $|\psi_i\rangle$  of the center-of-mass motion. Since  $\hat{U}_1$  is a unitary operator with  $\hat{U}_1^\dagger = \hat{U}_1^{-1}$  the expectation value e determining  $P_1$  enjoys a simple interpretation: we first evolve the state  $|\psi_i\rangle$  according to  $\hat{U}_u$  and then return to  $|\psi_i\rangle$  with the time-inverted evolution of  $\hat{U}_1$ . Since  $\hat{U}_1^{-1}\hat{U}_u$  is a unitary operator e must be a phase factor  $\exp(i\alpha)$ . However, we now show that already the operator product  $\hat{U}_1^\dagger \hat{U}_u$  is a e-number phase factor, that is we establish the identity

$$\hat{U}_{1}^{\dagger}\hat{U}_{1} = \hat{U}_{1}^{-1}\hat{U}_{1} = e^{i\alpha}. \tag{45}$$

The fact that this relation is independent of the representation is the deeper reason why the cancellation taking place in a specific representation cannot be relied on to draw conclusions about improved accuracy.

#### 4.2. Acceleration obtained from different sequences of events

We now derive explicit expressions for  $\hat{U}_u$  and  $\hat{U}_1$ . For this purpose we recall that the center-of-mass motion of an atom of mass m in a time-independent gravitational field of potential V = V(z) is governed by the time evolution operator

$$U_g \equiv \exp\left(-\frac{\mathrm{i}}{\hbar}\hat{H}T\right),\tag{46}$$

where

$$\hat{H} \equiv \frac{\hat{p}^2}{2m} + V(\hat{z}). \tag{47}$$

According to appendix A the action of the beam splitter can be described by the unitary operator

$$\hat{U}^{(\pm)}(t) \equiv e^{\pm i\left[k\hat{z} + \phi(t)\right]} \tag{48}$$

and  $\phi = \phi(t)$  denotes the phase of the laser pulse at time t.

When we substitute the expression (48) for  $\hat{U}^{(\pm)}$  into (41) and (42) for  $\hat{U}_{\rm u}$  and  $\hat{U}_{\rm l}$  we arrive at

$$\hat{U}_{u} = \hat{U}_{g} e^{-i[k\hat{z} + \phi(T)]} \hat{U}_{g} e^{i[k\hat{z} + \phi(0)]}$$
(49)

and

$$\hat{U}_{1} = e^{-i[k\hat{z} + \phi(2T)]} \hat{U}_{\varrho} e^{i[k\hat{z} + \phi(T)]} \hat{U}_{\varrho}.$$
(50)

Since the phases  $\phi(0)$ ,  $\phi(T)$  and  $\phi(2T)$  are c-numbers we can factor them out and we find the representation

$$\hat{U}_{u} = e^{i[-\phi(T) + \phi(0)]} \hat{U}_{g} \hat{U}_{g}^{(+)}$$
(51)

and

$$\hat{U}_1 = e^{i[-\phi(2T)+\phi(T)]} \hat{U}_g^{(+)} \hat{U}_g, \tag{52}$$

where we have introduced the abbreviation

$$\hat{U}_{\varrho}^{(+)} \equiv e^{-ik\hat{z}} e^{-i\hat{H}T/\hbar} e^{ik\hat{z}}$$
(53)

for the time evolution operator  $\hat{U}_g$  of the center-of-mass-motion of the atom in the gravitational field sandwiched between the two operators  $\exp(-\mathrm{i}k\hat{z})$  and  $\exp(\mathrm{i}k\hat{z})$  originating from the laser pulses.

With the help of the familiar techniques of operator algebra we rederive in appendix C the operator identity

$$\hat{U}_g^{(+)} \equiv \exp\left(-\frac{\mathrm{i}}{\hbar}\hat{H}^{(+)}T\right),\tag{54}$$

where

$$\hat{H}^{(+)} \equiv \frac{(\hat{p} + \hbar k)^2}{2m} + V(z) = \hat{H} + \frac{(\hbar k)^2}{2m} + \frac{\hbar k}{m} \hat{p}.$$
 (55)

In the last step we have recalled the definition (47) of  $\hat{H}$ .

Hence, the two paths in the interferometer correspond to two different orders of events: on the upper path we first propagate with an atom in  $|g_2\rangle$  and therefore with  $\hat{H}^{(+)}$ , and then with the atom  $|g_1\rangle$  which corresponds to the Hamiltonian  $\hat{H}$ . As a result we find

$$\hat{U}_{\mathbf{u}} = e^{i[-\phi(T) + \phi(0)]} \exp\left(-\frac{i}{\hbar}\hat{H}T\right) \exp\left(-\frac{i}{\hbar}\hat{H}^{(+)}T\right). \tag{56}$$

On the lower path we first propagate with the atom in  $|g_1\rangle$ , that is with  $\hat{H}$  and then with the atom in  $|g_2\rangle$  corresponding to  $\hat{H}^{(+)}$  which leads us to

$$\hat{U}_{1} = e^{i[-\phi(2T)+\phi(T)]} \exp\left(-\frac{i}{\hbar}\hat{H}^{(+)}T\right) \exp\left(-\frac{i}{\hbar}\hat{H}T\right). \tag{57}$$

The expressions (56) and (57) bring out most clearly the different sequence of events in the two arms of the interferometer by the different order of  $\hat{H}$  and  $\hat{H}^{(+)}$ .

The two Hamiltonians  $\hat{H}$  and  $\hat{H}^{(+)}$  do not commute with each other. Indeed, we find from (55) the identity

$$[\hat{H}, \hat{H}^{(+)}] = \frac{\hbar k}{m} [\hat{H}, \hat{p}] \tag{58}$$

which with the Heisenberg equations of motion

$$\dot{\hat{z}} = \frac{i}{\hbar}[\hat{H}, \hat{z}] = \frac{\hat{p}}{m} \quad \text{and} \quad \dot{\hat{p}} = m\ddot{\hat{z}} = \frac{i}{\hbar}[\hat{H}, \hat{p}],$$
 (59)

that is

$$m\ddot{\hat{z}} = \frac{\mathrm{i}}{\hbar}[\hat{H}, \,\hat{p}] \tag{60}$$

leads us to

$$[\hat{H}, \hat{H}^{(+)}] = -i\hbar^2 k \ddot{\hat{z}}. \tag{61}$$

Hence, the fact that  $\hat{H}$  and  $\hat{H}^{(+)}$  do not commute is a measure of the acceleration of the atom. We emphasize that so far we have not used the specific form of the potential. Indeed, the fact that the different order of  $\hat{H}$  and  $\hat{H}^{(+)}$  is a measure of the acceleration is true for any potential V = V(z) that is only dependent on position.

#### 4.3. Phase shift for linear gravitational potential

However, it is not straightforward to combine the two time evolutions due to  $\hat{H}$  and  $\hat{H}^{(+)}$  into a single one. Indeed, we recall the Baker–Cambell–Hausdorff theorem

$$e^{\hat{A}} e^{\hat{B}} = e^{\hat{A} + \hat{B}} e^{\frac{1}{2}[\hat{A}, \hat{B}]}, \tag{62}$$

which only holds true for

$$[\hat{A}, [\hat{A}, \hat{B}]] = [\hat{B}, [\hat{A}, \hat{B}]] = 0.$$
 (63)

However, for a constant gravitational field with a linear potential

$$V_g(z) \equiv mgz,\tag{64}$$

we find that the acceleration

$$\ddot{\hat{z}} = -g \tag{65}$$

is a c-number. As a result the conditions (63) are satisfied and we find from (62) for the Hamiltonians

$$\hat{H}_g \equiv \frac{\hat{p}^2}{2m} + mg\hat{z} \tag{66}$$

and

$$\hat{H}_g^{(+)} \equiv \frac{\left(\hat{p} + \hbar k\right)^2}{2m} + mg\hat{z},\tag{67}$$

the expressions

$$\hat{U}_{u} = e^{i[-\phi(T)+\phi(0)]} \exp\left[-\frac{1}{2} \left[\hat{H}_{g}, \hat{H}_{g}^{(+)}\right] \frac{T^{2}}{\hbar^{2}}\right] \exp\left[-\frac{i}{\hbar} \left(\hat{H}_{g} + \hat{H}_{g}^{(+)}\right) T\right]$$
(68)

and

$$\hat{U}_{1} = e^{i[-\phi(2T)+\phi(T)]} \exp\left[-\frac{1}{2} \left[\hat{H}_{g}^{(+)}, \hat{H}_{g}\right] \frac{T^{2}}{\hbar^{2}}\right] \exp\left[-\frac{i}{\hbar} \left(\hat{H}_{g}^{(+)} + \hat{H}_{g}\right) T\right].$$
 (69)

Indeed, with the help of the commutator (61) we arrive at the representations

$$\hat{U}_{II} = e^{i[-\phi(T) + \phi(0)]} e^{+i\delta\varphi/2} \hat{U}_{C}$$
(70)

and

$$\hat{U}_{1} = e^{i[-\phi(2T) + \phi(T)]} e^{-i\delta\varphi/2} \hat{U}_{c}$$
(71)

for the products  $\hat{U}_u$  and  $\hat{U}_1$  of the unitary operators along the upper and lower path. Here we have introduced the phase

$$\delta \varphi \equiv k \ddot{z} T^2 \tag{72}$$

which arises from the commutation relation (61) between  $\hat{H}_g$  and  $\hat{H}_g^{(+)}$  and contains the acceleration of the atom. Moreover, we have defined the unitary operator  $\hat{U}_c \equiv \exp[-\mathrm{i}(\hat{H}_g^{(+)} + \hat{H}_g)T]$  involving the sum of  $\hat{H}_g^{(+)}$  and  $\hat{H}_g$  and representing the time evolution due to both Hamiltonians.

Since  $\hat{H}_g + \hat{H}_g^{(+)} = \hat{H}_g^{(+)} + \hat{H}_g$  we find that  $\hat{U}_c$  appears identically in  $\hat{U}_u$  as well as  $\hat{U}_1$ . In addition on the upper path the phase shift  $\delta \varphi/2$  due to the acceleration appears with a plus sign whereas on the lower path occurs with a negative sign. Hence, we find a non-vanishing phase difference  $\delta \varphi$  between the two arms due to the acceleration of the atom.

#### 4.4. Phase shift caused by accelerations of the laser phase and atom

We are now in the position to prove our initial claim that the operator product  $\hat{U}_1^{\dagger}\hat{U}_u$  is a c-number phase factor. Indeed, with the help of (70) and (71) we immediately establish the identity

$$\hat{U}_{1}^{\dagger}\hat{U}_{u} = e^{i\alpha},\tag{73}$$

that is  $\hat{U}_1^\dagger \hat{U}_{\mathrm{u}}$  is free of any operators but only involves the sum

$$\alpha \equiv \delta\phi + \delta\varphi \tag{74}$$

of the phase difference  $\delta \phi$  between the phases of the laser pulses at the three interactions times, and the phase  $\delta \varphi$  due to the acceleration of the atom in the gravitational field. Here we have recalled the definition (26) of  $\delta \phi$ .

For the special case of a constant acceleration given by (65) we find from equation (72) the expression

$$\delta\varphi = -\delta\varphi_g \equiv -kgT^2. \tag{75}$$

In summary, the difference in the order of the time evolution operators  $\hat{H}_g$  and  $\hat{H}_g^{(+)}$  gives rise to a c-number phase factor  $\exp(-\mathrm{i}\delta\varphi_g)$  which is a measure of the acceleration of the atom in the gravitational potential. Another contribution to the phase shift  $\alpha$  in the interferometer arises from the phases  $\phi(0)$ ,  $\phi(T)$  and  $\phi(2T)$  of the laser pulses which appear in the expressions (56) and (57) for  $\hat{U}_u$  and  $\hat{U}_1$ . The sum of  $\delta\phi$  and  $\delta\varphi$  yields  $\alpha$  in complete agreement with the previous section.

It is interesting to note that (58) also suggests that the phase shift  $\delta \varphi$  is a consequence of the commutation relation

$$[\hat{p}, \hat{z}] = \frac{\hbar}{i}.\tag{76}$$

Indeed, with the definition (66) of  $\hat{H}_g$  we find from (58) the identity

$$[\hat{H}_g, \hat{H}_g^{(+)}] = \hbar kg [\hat{z}, \hat{p}] = i\hbar^2 kg$$
 (77)

which by virtue of (68), (69) and (75) yields again  $\delta \varphi_g$ .

#### 4.5. Summary of operator approach

In the present section we have developed a formalism based on unitary operators to obtain the phase shift in the Kasevich–Chu interferometer. Our representation-free approach brings out most clearly that this phase shift consists of the sum of only two phases: (i) the phase difference  $\delta \phi$  between the phases of the laser pulses at the three interaction times, and (ii) the phase  $\delta \varphi$  due to the acceleration of the atom in the gravitational field.

This result is in sharp contrast to the discussion in section 3.5 based on semiclassical considerations in position space which interprets the total phase shift as the sum of *four* phases with the cancellation of two. In the next section we shall show that this decomposition into the *two* phases  $\delta \phi$  and  $\delta \varphi$  is crucial in understanding the observed phase shift when we use different coordinate systems to describe the interferometer.

Moreover, our analysis also clearly shows that the phase shift depends on the specific interferometer configuration. Indeed, the unitary operators corresponding to the individual path

are determined by the sequence of beam splitters, mirrors, and motion in the gravitational field. It is the order of these events which gives rise to the phase shift.

We conclude by emphasizing that our operator approach toward atom interferometry is rather general and by no means limited to the Kasevich-Chu interferometer. Indeed, it can be applied to any other interferometer configuration.

Most recently, we have employed [64] this formalism to analyze the similarities and differences between an atom interferometer where the mirrors at t = T are realized by an evanescent light wave and the Kasevich–Chu interferometer. Such a device is motivated by analogies [51] between atom and neutron interferometers.

#### 5. Interplay between chirp and acceleration: different frames

The important roles of  $\delta \phi$  and  $\delta \varphi$  and their interplay in contributing to the total phase shift  $\alpha \equiv \delta \phi + \delta \varphi$  in the interferometer stand out most clearly in three scenarios summarized in table 2. So far we have concentrated on describing the interferometer in a frame in which the lasers and the observer are at rest and the atoms are accelerated by the gravitational field giving rise to the phase shift  $\delta \varphi = -\delta \varphi_g$ . For the sake of simplicity we assume that the phases of the laser pulse are constant in time and therefore,  $\delta \phi$  vanishes. Hence, the total phase shift  $\alpha$  in the interferometer solely results from the acceleration of the atom, that is  $\alpha = 0 + (-\delta \varphi_g) = -\delta \varphi_g$ . For this reason we refer to this scenario as the accelerometer scenario (I).

However, we can also describe this scenario in a frame in which the atoms are not accelerated. Since in this frame  $\ddot{z}=0$  the phase  $\delta\varphi$  given according to (72) by the acceleration of the atom vanishes.

This coordinate system is accelerated and as a result the phases of the laser pulses which are constant in the laboratory frame are not constant anymore but vary quadratically in time. Indeed, the Galilei-coordinate transformation

$$z_a \equiv z - \left(v_a t + \frac{1}{2}at^2\right) \tag{78}$$

connecting the z-coordinates z and  $z_a$  in the laboratory system and a frame accelerated with constant acceleration a and with the velocity  $v_a$  at t=0 transforms the phase of the electromagnetic wave to

$$kz + \phi(t) = k\left(z_a + v_a t + \frac{1}{2}at^2\right) + \phi(t) \equiv kz_a + \phi_a(t),$$
 (79)

where

$$\phi_a(t) \equiv \phi(t) + k \left( v_a t + \frac{1}{2} a t^2 \right) \tag{80}$$

denotes the phase of the pulse in the accelerated frame.

When we assume that in the laboratory frame  $\phi$  is time-independent we find

$$\ddot{\phi_a}(0) = ka,\tag{81}$$

which for a = -g leads to

$$\delta\phi = -kgT^2 = -\delta\varphi_g. \tag{82}$$

Hence, in the accelerated frame the total phase shift  $\alpha$  in the interferometer solely results from the quadratic variation of the laser pulse, that is from the chirp due to the coordinate

**Table 2.** Origin of the total phase shift  $\alpha$  in the Kasevich–Chu atom interferometer in three different scenarios each analyzed in the laboratory and in an accelerated frame. The total phase shift  $\alpha$  in the interferometer is given by the sum  $\alpha \equiv \delta \phi + \delta \varphi$  of the phases  $\delta \phi \equiv \phi(2T) - 2\phi(T) + \phi(0) \cong \ddot{\phi}(0)T^2$ and  $\delta \varphi \equiv k\ddot{z}T^2$  due to the accelerations  $\ddot{\varphi}$  and  $\ddot{z}$  of the laser phase and the atom in the gravitational field or from both giving rise to a vanishing of  $\alpha$ . The three scenarios referred to as accelerometer (I), inertial motion (II), and Einstein equivalence principle (III) are best described in the laboratory frame (lf): I—constant laser phase and gravity; II—constant laser phase and no gravity; and III—quadratic chirp of laser phase and gravity. We also analyze each scenario from an accelerated frame (af) which in I, II, and III are a = -g, g, and -g, respectively. We obviously arrive at the same answer for the total phase  $\alpha$  as in the laboratory frame. However,  $\alpha$  arises from different physical phenomena, either from the laser phase or the gravitational field. We emphasize that the analysis in the accelerated frame of scenario II is identical to the laboratory frame of scenario III which is a manifestation of the Einstein equivalence principle. Likewise, the laboratory frame of II is identical to the accelerated frame of III.

Scenarios	Frame used in analysis	Accelerations of coordinate system and atom	Phase $\delta \phi$ due to acceleration of pulses	Phase $\delta \varphi$ due to acceleration of atom	Total Phase $\alpha \equiv \delta \phi + \delta \varphi$
	lf	a = 0 $g$	0	$-\delta arphi_g$	$-\delta arphi_g$
Accelerometer (I)	${ m af}$	a = -g	$-\delta arphi_g$	0	$-\delta arphi_g$
Inertial	lf	•	0	0	0
motion (II)	af	<u> </u>	$\delta arphi_g$	$-\delta arphi_g$	0
Einstein equivalence	lf		$\delta arphi_g$	$-\delta arphi_g$	0
principle (III)	af	•	0	0	0

transformation (78). Indeed, we find  $\alpha = -\delta \varphi_g + 0 = -\delta \varphi_g$ , in complete agreement with the description in the laboratory frame.

A particularly instructive scenario arises when there is no gravity in the laboratory frame and the phases of the pulses are constant. We refer to this scenario as the inertial motion (II). In this case both phases  $\delta \phi$  and  $\delta \varphi$  vanish leading to  $\alpha = 0 + 0 = 0$ .

However, when we describe the situation in a frame that is accelerated with a=g so that it looks like the atom is in a gravitational field the phases of the atom as well as of the laser are non-vanishing. Indeed, for the atom it is as if the gravity is leading again to  $\delta\varphi=-\delta\varphi_g$  while the laser phase gets chirped giving rise according to (81) to  $\delta\phi=kgT^2=\delta\varphi_g$ . However, both effects compensate each other in the total phase  $\alpha=\delta\varphi_g+(-\delta\phi_g)=0$ , in complete agreement with the description in the laboratory frame.

The understanding of the third scenario referred to as Einstein equivalence principle is crucial for the experiments discussed in [36, 38–52]. In these experiments the laser fields are chirped in the laboratory frame in a way to compensate for the phase shift  $\delta \varphi = -\delta \varphi_g$  due to the gravitational field, that is  $\delta \varphi = -\delta \varphi = \delta \varphi_g$  which yields indeed  $\alpha = \delta \varphi_g + (-\delta \varphi_g) = 0$ . Therefore, this situation corresponds to the inertial-motion scenario II viewed from the accelerated frame.

For the sake of completeness we also briefly mention a description of scenario III in which the coordinate system is accelerated with the atom, that is a=-g. In this frame the chirped pulse has a constant phase, that is  $\delta \phi = 0$ . Moreover, the phase  $\delta \varphi$  due to the acceleration of the atom vanishes as well, leading to  $\alpha = 0 + 0 = 0$ , in complete accordance with the previous analysis of scenario III.

#### 6. Phase shift obtained in momentum representation

The operator approach of section 4 brings out most clearly that the product  $\hat{U}_1^{\dagger}\hat{U}_u$  of unitary operators determining in (44) the probability  $P_1$  of an atom to be at the exit of the interferometer in  $|g_1\rangle$  reduces to a c-number phase factor. This phase factor is an observable.

Needless to say, we do not have to resort to operator algebra to evaluate the operator product. We might as well have used a specific representation of the center-of-mass motion. In the present and the next section we analyze the atom interferometer using two representations: first the momentum and then the position representation.

We start our discussion by considering the momentum representation and show that in this formulation the contribution  $\delta \varphi_g$  to the total phase shift  $\alpha$  in the interferometer arises solely from the unitary time evolution of the momentum eigenstates between the laser pulses. For this purpose we represent the operator product

$$\hat{U}_{1}^{\dagger}\hat{U}_{u} = \int_{-\infty}^{\infty} dp' \int_{-\infty}^{\infty} dp \langle p' | \hat{U}_{1}^{\dagger} \hat{U}_{u} | p \rangle | p' \rangle \langle p |$$
(83)

in terms of momentum eigenstates  $|p\rangle$  and thus have to evaluate the action of  $\hat{U}_u$  and  $\hat{U}_1$  on  $|p\rangle$ . With the help of (49) and (50) we obtain the explicit expressions

$$\hat{U}_{\mathbf{u}}|p\rangle = e^{-i\hat{H}_g T/\hbar} e^{-i\left[k\hat{z} + \phi(T)\right]} e^{-i\hat{H}_g T/\hbar} e^{i\left[k\hat{z} + \phi(0)\right]}|p\rangle$$
(84)

and

$$\hat{U}_{1}|p\rangle = e^{-i\left[k\hat{z}+\phi(2T)\right]} e^{-i\hat{H}_{g}T/\hbar} e^{i\left[k\hat{z}+\phi(T)\right]} e^{-i\hat{H}_{g}T/\hbar}|p\rangle, \tag{85}$$

where we have used the definition (46) of  $\hat{U}_g$  and have replaced  $\hat{H}$  by  $\hat{H}_g$ .

#### 6.1. Propagation in the gravitational potential

Next we recall the familiar relation

$$e^{\pm ik\hat{z}}|p\rangle = |p \pm \hbar k\rangle \tag{86}$$

shifting  $|p\rangle$  by  $\pm \hbar k$  where the plus or minus signs correspond to the absorption or emission of the photon, respectively. We emphasize that here the signs are opposite to but consistent with the ones in the definition (11) of  $V_{lp}$ . The reason for this counter-intuitive fact stands out most clearly from appendix A.5 which allows us trace this sign change back to the fact that time evolution in quantum mechanics is always given by  $\exp(-i\hat{H}t/\hbar)$ .

Moreover, in appendix D we verify the identity

$$e^{-i\hat{H}_g t/\hbar} |p_g(0)\rangle = e^{-i[\kappa(p_g(0)) - \kappa(p_g(t))]} |p_g(t)\rangle$$
(87)

with

$$p_g(t) \equiv p_g(0) - mgt \tag{88}$$

and

$$\kappa(p) \equiv \frac{p^3}{6\hbar m^2 g}.\tag{89}$$

Equation (87) states that during the time evolution in a linear gravitational potential a momentum eigenstate  $|p_g(0)\rangle$  remains a momentum eigenstate and its eigenvalue follows Newtonian dynamics. However, the state also acquires a phase which is the difference of the phases evaluated at the initial and the final momentum, that is the difference between  $\kappa$  at  $p_g(0)$  and  $\kappa$  at  $p_g(t)$ . It is also interesting that  $\kappa$  is cubic in the momentum.

With the help of the identities (86) and (87) we find for the actions of the unitary operators  $\hat{U}_{\rm u}$  and  $\hat{U}_{\rm l}$  corresponding to the upper and the lower paths on the initial momentum state  $|p_g(0)\rangle$  the expressions

$$\hat{U}_{u}|p_{g}(0)\rangle = e^{i[-\phi(T)+\phi(0)]} e^{-i\Delta_{u}}|p_{g}(2T)\rangle$$
(90)

and

$$\hat{U}_1 | p_g(0) \rangle = e^{i[-\phi(2T) + \phi(T)]} e^{-i\Delta_1} | p_g(2T) \rangle$$
(91)

with the phases

$$\Delta_{\mathbf{u}} \equiv \kappa(p_{g}(T)) - \kappa(p_{g}(2T)) + \kappa(p_{g}(0) + \hbar k) - \kappa(p_{g}(T) + \hbar k) \tag{92}$$

and

$$\Delta_1 \equiv \kappa(p_{\varrho}(T) + \hbar k) - \kappa(p_{\varrho}(2T) + \hbar k) + \kappa(p_{\varrho}(0)) - \kappa(p_{\varrho}(T)). \tag{93}$$

Hence, on both paths the propagation of the initial momentum state  $|p_g(0)\rangle$  by  $\hat{U}_u$  and  $\hat{U}_1$  leads to the same momentum state  $|p_g(2T)\rangle = |p_g(0) - mg(2T)\rangle$  which differs from  $|p_g(0)\rangle$  due its motion in the gravitational field. In particular,  $|p_g(2T)\rangle$  is independent of the momentum kicks  $\pm \hbar k$  originating from the interaction of the atom with the laser pulses since on both paths one photon is first absorbed but then again emitted. Moreover, the phases  $\phi(0)$ ,  $\phi(T)$  and  $\phi(2T)$  appear in the same way as in the operator approach, a fact which is not surprising since they are c-numbers.

#### 6.2. Diagonal representation of operator product due to identical final states

In the evaluation of the matrix element  $\langle p'|\hat{U}_1^{\dagger}\hat{U}_u|p\rangle$  we need for  $\hat{U}_1$  the initial momentum state  $|p'\rangle$  rather than  $|p\rangle$ . Thus we arrive at the final momentum state  $|p'(2T)\rangle = |p'(0) - 2mgT\rangle$  rather than  $|p_g(2T)\rangle = |p_g(0) - 2mgT\rangle$  and the initial momentum  $p_g(0)$  is replaced by  $p_g'(0)$ . Likewise, we need to substitute in  $\Delta_1$  the momentum  $p_g(0)$  by  $p_g'(0)$  which we denote by a prime on  $\Delta_1$ , that is  $\Delta_1'$ .

From (90) and (91) we find that the matrix element

$$\langle p_g'(0)|\hat{U}_1^{\dagger}\hat{U}_u|p_g(0)\rangle = e^{i\delta\phi} e^{-i(\Delta_u - \Delta_1')} \langle p_g'(2T)|p_g(2T)\rangle$$
 (94)

consists of the product of two phase factors and the scalar product

$$\langle p_g'(2T)|p_g(2T)\rangle = \langle p_g'(0) - 2mgT|p_g(0) - 2mgT\rangle \tag{95}$$

between two momentum states. Here we have also recalled the definition (26) of  $\delta \phi$ .

The orthonormality condition  $\langle p'|p\rangle = \delta(p'-p)$  of momentum states reduces (94) to

$$\langle p_g'(0)|\hat{U}_1^{\dagger}\hat{U}_u|p_g'(0)\rangle = e^{i\delta\phi} e^{-i(\Delta_u - \Delta_l)} \delta(p_g'(0) - p_g(0)). \tag{96}$$

Here we have already made use of the delta function to replace  $\Delta'_1$  by  $\Delta_1$ .

The phase difference  $\Delta \equiv \Delta_u - \Delta_l$  between the upper and the lower path is given by the difference

$$\Delta \equiv \delta \kappa (p_{g}(0)) - \delta \kappa (p_{g}(0) + \hbar k) \tag{97}$$

between the quantity

$$\delta\kappa(p_{\varrho}(0)) \equiv \kappa(p_{\varrho}(2T)) - 2\kappa(p_{\varrho}(T)) + \kappa(p_{\varrho}(0)) \tag{98}$$

evaluated at  $p_g(0)$  and  $p_g(0) + \hbar k$ .

When we substitute (96) into the momentum representation (83) of  $\hat{U}_1^{\dagger}\hat{U}_u$  we obtain by performing the integration over p' with the help of the delta function the identity

$$\hat{U}_{l}^{\dagger}\hat{U}_{u} = e^{i\delta\phi} \int_{-\infty}^{\infty} dp_{g}(0) e^{-i\Delta} |p_{g}(0)\rangle\langle p_{g}(0)|, \qquad (99)$$

that is  $\hat{U}_{1}^{\dagger}\hat{U}_{u}$  is diagonal.

#### 6.3. The phase shift in the interferometer is independent of the momentum

Unfortunately, the definition (97) of  $\Delta$  suggests that  $\Delta$  depends on  $p_g(0)$  and we cannot yet use the completeness relation to arrive at the desired phase factor representation (73) of the operator product. However, we now show that  $\Delta$  is indeed independent of  $p_g(0)$ .

For this purpose we first note that in complete analogy to  $\delta \phi$  also  $\delta \kappa$  involves the times 0, T and 2T of the laser pulses and is of the form of the discrete version of a second derivative in time, that is

$$\delta\kappa(p_g(0)) \cong \frac{\mathrm{d}^2}{\mathrm{d}t^2}\kappa(p_g(t))|_{t=0}T^2 = \left.\frac{\partial^2\kappa}{\partial p^2}\right|_{p=p_g(0)} \left(\frac{\partial p_g}{\partial t}\right)^2\Big|_{t=0}T^2. \tag{100}$$

In the last step we have made use of the fact that in a constant gravitational field the second derivative of the momentum vanishes.

When we replace the difference of momenta in  $\Delta$  by the differential, that is

$$\Delta \cong -\frac{\partial}{\partial p} (\delta \kappa) \hbar k, \tag{101}$$

we find with the help of (100) as well as the definitions (88) and (89) of  $p_g$  and  $\kappa$  the result

$$\Delta = -\left. \frac{\partial^3 \kappa}{\partial p^3} \right|_{p=p_g(0)} \left( \frac{\partial p_g}{\partial t} \right)^2 \bigg|_{t=0} \hbar k T^2 = -gkT^2 = -\delta \varphi_g. \tag{102}$$

We emphasize that (100) and (101) are exact as can easily be verified by evaluating the full expressions.

Equation (102) shows that  $\Delta$  is independent of  $p_g(0)$  and (99) reduces to

$$\hat{U}_1^{\dagger} \hat{U}_{\mathbf{u}} = e^{\mathrm{i}\alpha} \int_{-\infty}^{\infty} \mathrm{d}p_g(0) |p_g(0)\rangle \langle p_g(0)| = e^{\mathrm{i}\alpha}, \tag{103}$$

where we have recalled the definition (35) of  $\alpha$  and taken once again advantage of the completeness relation of the momentum states.

#### 6.4. Summary

In this section we have rederived from the momentum representation of quantum mechanics the result (73) that the operator product  $\hat{U}_l^\dagger \hat{U}_u$  is a c-number phase factor. Our calculation rests on three facts: (i) the time evolution of a momentum eigenstate along the two arms of the interferometer leads to the same final momentum state which ensures that the momentum representation of  $\hat{U}_l^\dagger \hat{U}_u$  is diagonal; (ii) the phase difference  $\Delta$  accumulated by the momentum states in the gravitational field between the laser pulses is the difference of  $\delta \kappa$  at the momenta p and  $p + \hbar k$  where  $\delta \kappa$  contains the momenta at the times of the three laser pulses which equates  $\Delta$  to  $\delta \varphi_g$ ; (iii) hence,  $\Delta$  is independent of the initial momentum which reduces  $\hat{U}_l^\dagger \hat{U}_u$  to a phase factor.

Our calculation suggests that the phase shift  $\alpha$  in the Kasevich–Chu interferometer is determined by the difference between the acceleration-like chirp of the phases of the laser pulses and the phase difference between the dynamical phases acquired by the atom in the two arms during its motion in the gravitational field.

#### 7. Phase shift obtained in position representation

We now analyze the interferometer in position space and arrive at a description [52] in terms of propagators and the Feynman path integral. However, in contrast to [39, 41, 52] which start from this formulation of quantum mechanics we perform the complete calculation in standard non-relativistic Schrödinger quantum mechanics. Needless to say during our analysis we shall repeatedly make contact with the Feynman approach.

As motivated by the previous sections we focus on the operator product  $\hat{U}_{l}^{\dagger}\hat{U}_{u}$  and represent it now in terms of position eigenstates  $|z\rangle$ . With the help of the completeness relation we find

$$\hat{U}_{1}^{\dagger}\hat{U}_{u} = \int_{-\infty}^{\infty} dz''' \int_{-\infty}^{\infty} dz \ M(z''', z) |z'''\rangle\langle z|, \tag{104}$$

where we have introduced the matrix element

$$M \equiv \langle z'''|\hat{U}_1^{\dagger}\hat{U}_u|z\rangle = \int_{-\infty}^{\infty} dz'' \langle z'''|\hat{U}_1^{\dagger}|z''\rangle \langle z''|\hat{U}_u|z\rangle$$
 (105)

consisting of the product of the matrix elements  $\langle z''|\hat{U}_{\rm u}|z\rangle$  and  $\langle z'''|\hat{U}_{\rm l}^{\dagger}|z''\rangle = \langle z''|\hat{U}_{\rm l}|z'''\rangle^*$  representing the propagation from z to z'' according to the unitary evolution operator  $\hat{U}_{\rm u}$ , and the reverse motion from z'' to z''' due to  $\hat{U}_{\rm l}^{\dagger}$ . In order to obtain M which connects z with z''' we have to integrate over the intermediate coordinate z''.

#### 7.1. Propagation on a continuum of paths

We start by evaluating the action of  $\hat{U}_u$  and  $\hat{U}_1$  on a position eigenstate  $|z\rangle$ . Unfortunately, the time evolution of  $|z\rangle$  in a linear potential is slightly more complicated than that of  $|p\rangle$ . In particular,  $|z\rangle$  does not remain an eigenstate.

We calculate the matrix elements  $\langle z''|\hat{U}_{\rm u}|z\rangle$  and  $\langle z''|\hat{U}_{\rm l}|z'''\rangle$  with the help of the expressions (49) and (50) for  $\hat{U}_{\rm u}$  and  $\hat{U}_{\rm l}$  by inserting a complete set of states  $|z'\rangle$  and  $|\tilde{z}'\rangle$ . In particular, we find the representation

$$\langle z''|\hat{U}_{\mathbf{u}}|z\rangle = \int_{-\infty}^{\infty} dz' \langle z''|e^{-i\hat{H}_gT/\hbar}|z'\rangle \langle z'|e^{-i[k\hat{z}+\phi(T)]}e^{-i\hat{H}_gT/\hbar}e^{i[k\hat{z}+\phi(0)]}|z\rangle.$$
(106)

Here we have replaced in  $\hat{U}_g$  the Hamiltonian  $\hat{H}$  by  $\hat{H}_g$ , that is we consider again for the sake of clarity the case of a constant gravitational field.

The familiar identity

$$e^{\pm ik\hat{z}}|z\rangle = e^{\pm ikz}|z\rangle \tag{107}$$

leads us to the expression

$$\langle z''|\hat{U}_{u}|z\rangle = \int_{-\infty}^{\infty} dz' \, G(z'', T|z') \, e^{-i[kz'+\phi(T)]} \, G(z', T|z) \, e^{i[kz+\phi(0)]}, \tag{108}$$

where we have introduced the propagator  $G(z', T|z) \equiv \langle z'| \mathrm{e}^{-\mathrm{i}\hat{H}_g T/\hbar}|z\rangle$  in the linear gravitational field which takes the atom during the time T from the position z to z'. Moreover, we have left the terms in the sequence in which they appear on the upper path.

Similarly, we arrive with the representation (50) of  $\hat{U}_1$  at

$$\langle z''|\hat{U}_1|z'''\rangle = \int_{-\infty}^{\infty} d\tilde{z}' \langle z''|e^{-i[k\hat{z}+\phi(2T)]} e^{-i\hat{H}_gT/\hbar} |\tilde{z}'\rangle \langle \tilde{z}'|e^{i[k\hat{z}+\phi(T)]} e^{-i\hat{H}_gT/\hbar} |z'''\rangle, \tag{109}$$

that is

$$\langle z''|\hat{U}_1|z'''\rangle = \int_{-\infty}^{\infty} d\tilde{z}' \, e^{-i[kz'' + \phi(2T)]} \, G(z'', T|\tilde{z}') \, e^{i[kz' + \phi(T)]} \, G(\tilde{z}', T|z'''). \tag{110}$$

For a linear potential the propagator G which contains the classical action

$$S_{\rm cl}(z', T|z) \equiv \frac{m}{2T}(z'-z)^2 - \frac{1}{2}(z+z')mgT - \frac{1}{24}mg^2T^3$$
 (111)

corresponding to the Newtonian trajectory connecting during the time T the two positions z and z', and a normalization factor

$$N \equiv \sqrt{\frac{m}{2\pi i\hbar T}} \tag{112}$$

which depends on T but not on z or z', takes the form

$$G(z', T|z) = N \exp\left[\frac{i}{\hbar} S_{cl}(z', T|z)\right]. \tag{113}$$

As a result the matrix element corresponding to the upper path reads

$$\langle z''|\hat{U}_{\mathbf{u}}|z\rangle = e^{\mathbf{i}[-\phi(T)+\phi(0)]} N^2 \int_{-\infty}^{\infty} dz' \exp\left[\frac{\mathbf{i}}{\hbar} \Lambda_{\mathbf{u}}(z'; z'', z)\right], \tag{114}$$

where

$$\Lambda_{\rm u}(z';z'',z) \equiv S_{\rm cl}(z'',T|z') + S_{\rm cl}(z',T|z) + \hbar k(-z'+z). \tag{115}$$

In (114) the integration over the coordinate z' constitutes an integration over paths. Indeed, the appearance of the sum of the two classical actions  $S_{\rm cl}(z'',T|z')$  and  $S_{\rm cl}(z',T|z)$  in (115) indicates that we start at z and reach z'' on a continuum of paths given by all possible intermediate coordinates z' ranging from minus to plus infinity. The expression (114) is the Feynman path integral for the matrix element  $\langle z''|\hat{U}_{\rm u}|z\rangle$ .

Likewise, we find from (110) for the lower path

$$\langle z''|\hat{U}_1|z'''\rangle = e^{i[-\phi(2T)+\phi(T)]} N^2 \int_{-\infty}^{\infty} d\tilde{z}' \exp\left[\frac{i}{\hbar} \Lambda_1(\tilde{z}'; z'', z''')\right]$$
(116)

with

$$\Lambda_{1}(\tilde{z}'; z'', z''') \equiv S_{cl}(z'', T|\tilde{z}') + S_{cl}(\tilde{z}', T|z''') + \hbar k(-z'' + \tilde{z}'). \tag{117}$$

The integration variables z' and  $\tilde{z}'$  enter into  $\Lambda_u$  and  $\Lambda_1$  through the actions  $S_{cl}$  in the same way. However, in  $\Lambda_u$  the term  $\hbar kz'$  appears with a negative sign, corresponding to the emission of a photon of momentum  $\hbar k$  due to the second laser pulse, whereas at  $\Lambda_1$  the contribution  $\hbar k\tilde{z}'$  carries a positive sign representing absorption. Needless to say, this difference in signs makes a decisive difference in the integrals defining the two matrix elements. Hence, each trajectory characterized by the start and end points z and z'', or by z''' and z'' respectively but most importantly by the mid points z' and  $\tilde{z}'$ , carries a phase  $\Lambda_u/\hbar$  or  $\Lambda_1/\hbar$ . They depend not only on these coordinates but also on the path the atom has taken as expressed by the subscripts u and u.

#### 7.2. Matrix element

We are now in the position to evaluate the matrix element M given by (105). For this purpose we substitute (114) and (116) into (105) and find

$$M = e^{i\delta\phi} |N|^4 \int_{-\infty}^{\infty} dz'' \int_{-\infty}^{\infty} dz' \int_{-\infty}^{\infty} d\tilde{z}' \exp\left\{\frac{i}{\hbar} \left[\Lambda_{\mathrm{u}}(z'; z'', z) - \Lambda_{\mathrm{l}}(\tilde{z}'; z'', z''')\right]\right\}. \tag{118}$$

Here we have recalled the definition (26) of  $\delta \phi$ .

It is interesting to note that M is a triple integral of a phase factor whose phase is given by the difference  $\Lambda_{\rm u}-\Lambda_{\rm l}$  between the phases accumulated on the upper and the lower arm of the interferometer. The three integration variables are the three coordinates given by the intermediate points z and  $\tilde{z}'$  on the upper and the lower path and the end point z'' of both arms. We emphasize that at this stage we do not yet know that the path is closed. Indeed, we have not shown that z=z''', that is the property of the operator product  $\hat{U}_1^{\dagger}\hat{U}_u$  being diagonal.

In order to achieve this goal, two approaches offer themselves: we can take advantage of the fact that z' only enters into  $\Lambda_u$ , and  $\tilde{z}'$  only into  $\Lambda_1$  and perform the integrations separately. Since  $\Lambda_u$  and  $\Lambda_1$  contain the integration variables z' and  $\tilde{z}'$  at most quadratically the required integrations can be evaluated in an exact way. Moreover, this technique allows us to make contact with the classical trajectories and actions analyzed in section 3. However, there is a slight complication due to the fact that we do not know yet that  $\hat{U}_1^{\dagger}\hat{U}_u$  is diagonal and thus  $z \neq z'''$ . As a result the integrations do not yield as much insight as one would want.

For this reason we follow a different route and first perform the integration over z''. In appendix  $\mathbf{E}$  we include for the sake of completeness the detailed analysis of the first approach.

#### 7.3. Interference of end points yields coupling of the two arms

When we recall the definitions (115) and (117) of  $\Lambda_u$  and  $\Lambda_l$  the matrix element M given by (118) takes the form

$$M = e^{i\delta\phi} \frac{m}{2\pi\hbar T} \int_{-\infty}^{\infty} dz' \int_{-\infty}^{\infty} d\tilde{z}' I(\tilde{z}', z') \times \exp\left\{\frac{i}{\hbar} \left[S_{cl}(z', T|z) - S_{cl}(\tilde{z}', T|z''') + \hbar k(z - z' - \tilde{z}')\right]\right\},$$
(119)

where we have introduced the integral

$$I \equiv \frac{1}{2\pi} \frac{m}{\hbar T} \int_{-\infty}^{\infty} dz'' \exp\left\{\frac{i}{\hbar} \left[ S_{cl}(z'', T|z') - S_{cl}(z'', T|\tilde{z}') + \hbar k z'' \right] \right\}$$
(120)

and have recalled the definition (112) of the normalization constant N.

The explicit form (111) of  $S_{cl}$  reduces I to

$$I(\tilde{z}',z') = \frac{1}{2\pi} \int_{-\infty}^{\infty} dK \exp\left[i\left(\tilde{z}'-z'+\frac{\hbar k}{m}T\right)K\right] \times \exp\left\{-i\frac{m}{2\hbar T}(\tilde{z}'-z')\left[\tilde{z}'+z'-gT^2\right]\right\},\tag{121}$$

where we have introduced the integration variable  $K \equiv mz''/(\hbar T)$ .

Hence, the integral over z'', that is over K, is the Fourier representation of a delta function and we arrive at

$$I = \delta \left( \tilde{z}' - z' + \frac{\hbar k}{m} T \right) \exp \left[ ik \left( z' - \frac{\hbar k}{2m} T - \frac{1}{2} g T^2 \right) \right], \tag{122}$$

where we have used the familiar property

$$f(x)\delta(x) = f(0)\delta(x). \tag{123}$$

As a result, the integration over all end points z'', that is the interference of all paths leading to the same end point z'' has resulted in a delta function which couples the mid points z' and  $\tilde{z}'$  of the two integrations. Indeed, the relation

$$z' = \tilde{z}' + \frac{\hbar k}{m}T\tag{124}$$

indicates that the mid point z' on the upper arm is separated from the one on the lower arm, that is from  $\tilde{z}'$  by the distance  $\hbar kT/m$  traveled by the atom in the time T due to the momentum

transfer  $\hbar k$  resulting from the first laser pulse. This observation is in complete agreement with the lower part of table 1 which predicts the dependence

$$z_{\rm u} = z_{\rm l} + \frac{\hbar k}{m}t\tag{125}$$

for the time-dependent coordinates of the classical trajectories corresponding to the two arms.

Next we substitute the result (122) for I into (119) for M and perform with the help of the delta function the integration over  $\tilde{z}'$  which yields

$$M = e^{i\delta\phi} \frac{m}{2\pi\hbar T} \int_{-\infty}^{\infty} dz' \exp\left\{\frac{i}{\hbar} \left[ S_{cl}(z', T|z) - S_{cl}\left(z' + \frac{\hbar k}{m}T, T|z'''\right) + \hbar k \left(z - z' - \frac{1}{2}gT^2\right) \right] \right\}.$$

$$(126)$$

Now we are left with a single integration only and the definition (111) of  $S_{cl}$  finally leads us to

$$M = e^{i\alpha} \frac{1}{2\pi} \int_{-\infty}^{\infty} d\zeta \ e^{i(z-z''')\zeta} = e^{i\alpha} \delta(z - z'''), \tag{127}$$

where we have introduced the integration variable  $\zeta \equiv mz'/(\hbar T)$ .

Due to the delta function in the difference z - z''' arising from the integration over z', that is over  $\zeta$  the matrix element M is diagonal with the phase factor  $\exp(i\alpha)$  and reduces to

$$\hat{U}_1^{\dagger} \hat{U}_{\mathbf{u}} = \mathbf{e}^{\mathbf{i}\alpha},\tag{128}$$

in complete agreement with the representation-free approach based on operator algebra, or the momentum representation.

#### 7.4. Connection to semi-classical description

At this point it is useful to focus on the essential points of this rather lengthy calculation. Indeed, we identify the expression (118) for the matrix element M as the crucial quantity which contains three important ingredients. (i) It is determined by the integration of a phase factor over the mid points z' and  $\tilde{z}'$  as well as the end point z'' of the interferometer. (ii) The phase of the phase factor involves in the classical actions corresponding to the motion of the atom in the gravitational potential and the momentum exchange with the laser pulses the integration variables z',  $\tilde{z}'$  and z'' in a way such that the integration over all end points z'' enforces a constant separation  $\hbar kT/m$  between z' and  $\tilde{z}'$ . (iii) This constraint allows us to perform the integration over  $\tilde{z}'$ , and the resulting phase together with the integration over z' leads us to the diagonal nature of M, and thereby closes the path, that is z''' = z'.

We emphasize that at no point in this exact evaluation of the operator product  $\hat{U}_1^{\dagger}\hat{U}_u$  in position space did we take advantage of, or are even reminded of the cancellation of the dynamical phases associated with the kinetic and the potential energy which has played a key role in the semi-classical treatment of section 2. Indeed, these phases did not even appear in the final expression since parts of them were needed to perform the integrations over z',  $\tilde{z}'$  and z''. Hence, the exact evaluation of M in position space proceeds in quite a different manner than the semi-classical one. Needless to say we arrive at the same result.

In order to bring out most clearly the similarities and differences between the two approaches we first cast the exact expression (118) for M into the form

$$\langle z'''|\hat{U}_{1}^{\dagger}\hat{U}_{u}|z\rangle = |N|^{4} \int_{-\infty}^{\infty} dz'' \int_{-\infty}^{\infty} dz' \int_{-\infty}^{\infty} d\tilde{z}' \exp\left(\frac{i}{\hbar}S\right). \tag{129}$$

Here we have introduced the abbreviation

$$S \equiv S_{cl}(z''', T|\tilde{z}') + S_{cl}(\tilde{z}', T|z'') + S_{cl}(z'', T|z') + S_{cl}(z', T|z) + \hbar \left[kz'' + \phi(2T)\right] - \hbar \left[k\tilde{z}' + \phi(T)\right] - \hbar \left[kz' + \phi(T)\right] + \hbar \left[kz + \phi(0)\right]$$
(130)

and have also recombined the phases  $\phi(0)$ ,  $\phi(T)$  and  $\phi(2T)$  of the laser pulse with the phases kz, kz',  $k\tilde{z}'$  and kz'' of the atom in the laser. Since the interferometer has two arms we have two phases kz' and  $k\tilde{z}'$  at the time T.

Next we express the classical action  $S_{cl}$  of the atom in the linear gravitational potential given by (111) by the time integral of the corresponding Lagrangian  $\mathcal{L}_g$  defined by (19). In this way we can cast the quantity S determining M into the compact form

$$S = \int_{\mathcal{C}} dt \, \mathcal{L}_g - \int_{\mathcal{C}} dt \, V_{lp} \equiv \int_{\mathcal{C}} dt \, \mathcal{L}. \tag{131}$$

Here  $\mathcal{L}$  follows from (9) and  $\mathcal{C}$  denotes a path in time such that at the moments t=0, T and 2T of the laser pulses the coordinates z, z',  $\tilde{z}'$  and z'' together with the start points z and z''' define the path  $z \to z' \to z'' \to z'' \to z'''$  in position space. We evaluate the action corresponding to the Lagrangian  $\mathcal{L}$  along such a path.

The formal expression (131) for S brings (129) into the form

$$\langle z'''|\hat{U}_{1}^{\dagger}\hat{U}_{u}|z\rangle = \int \mathcal{D}\{z\} \exp\left(\frac{i}{\hbar} \int_{\mathcal{C}} dt \,\mathcal{L}\right),\tag{132}$$

where we have introduced the abbreviation

$$\int \mathcal{D}\{z\} \equiv |N|^4 \int_{-\infty}^{\infty} dz'' \int_{-\infty}^{\infty} dz' \int_{-\infty}^{\infty} d\tilde{z}'$$
(133)

for the three integrations.

The phase factor in the expression (132) for the matrix element  $\langle z'''|\hat{U}_1^{\dagger}\hat{U}_u|z\rangle$  is reminiscent of the semi-classical analysis of section 3. However, we emphasize that in the exact calculation discussed in the present section we have to integrate this phase factor over z'', z' and  $\tilde{z}'$ , that is we have to average it over a continuum of paths. The only points that are fixed in this average are the start and the end points z and z'' of these trajectories. In particular, this phase factor is not evaluated at the points z(2T),  $z'_u$  and  $z'_l$  given by the classical trajectories in contrast to the semi-classical one. Most importantly the path is not closed and  $z \neq z'''$ . A closed path emerges only after we have performed all three integrations. Obviously at this stage of the calculation the semi-classical phase factor in terms of  $\mathcal{L}$  does not exist anymore since we needed parts of it to perform the integrations.

Needless to say, the final expression for the phase shift derived from the exact calculation is identical to the one obtained from the semi-classical analysis. However, the way in which we arrive at this result is fundamentally different in the two approaches. This feature is just one more vivid demonstration that the procedures to evaluate the operator product depend on the representation, an observation which constitutes the central theme of our article.

#### 8. Summary and outlook

In summary, based on our operator approach we have shown that the phase shift in the Kasevich–Chu interferometer is the sum of only *two* phases which correspond to the acceleration of the phases of the laser pulses, and the acceleration of the atom. We have demonstrated that the latter term results from the difference in the order of two unitary time evolutions giving rise to a *c*-number phase factor in the interfering amplitudes corresponding to the two paths. When we evaluate the operator product determining the number of atoms at the exit ports in different representations we, of course, always arrive at the same phase factor. However, the way in which this term emerges depends critically on the representation. Therefore, in different representations the contributing terms appear to arise from different physical origins.

For example, in the momentum representation the phase due to the acceleration arises from the time evolution between the laser pulses. This behavior is in sharp contrast to the position representation where this phase results from the interference of a continuum of paths corresponding to a continuum of positions of the atom at the times of the laser pulses. This representation is intimately connected to the Feynman path integral approach in which the phase shift is solely the result of the interaction of the atom with the laser pulses. It is the difference of this interaction between the upper and lower beams that introduces gravity into the problem. Indeed, here the time evolution of the atom between the pulses is identical in the two arms and therefore cancels out in the relative phase.

Our operator approach confirms that the Kasevich–Chu interferometer is a accelerometer or a gravimeter [38, 39], but not an ensemble of two clocks. Moreover, due to the representation dependence of the phase shift there is no justification to prefer one representation over another. Therefore, conclusions drawn from one specific representation do not justify any claims concerning an improved accuracy.

#### **Acknowledgments**

We would like to thank Achim Peters and Holger Müller for explaining some of the subtle points of the atomic fountain experiments to us, and to Markus Aspelmeyer, Endre Kajari, Robert F O'Connell and Anton Zeilinger for discussions. Moreover, we are most grateful to Claude Cohen–Tannoudji for his critical reading of our article and for many useful comments. As part of the QUANTUS collaboration, this project was supported by the German Space Agency DLR with funds provided by the Federal Ministry of Economics and Technology (BMWi) under grant no. DLR 50 WM 0837. One of us (DMG) is grateful to the Alexander von Humboldt-Stiftung for a Wiedereinladung which made the start of this work possible, and to the Templeton Foundation for the grant # 21531, which allowed its completion.

#### Appendix A. Description of atom interferometer

In the present appendix we develop an elementary description of the Kasevich-Chu interferometer. For this purpose we study the interaction of a three-level atom with a short laser pulse and show that the resulting Schrödinger dynamics realizes a coherent beam splitter for the atomic motion. Here we first assume arbitrary transmission and reflection coefficients determined by the parameters of the laser pulses and then consider the special case of the

Kasevich–Chu interferometer. We conclude by deriving the effective potential  $V_{lp}$  for the center-of-mass-motion resulting from a short laser pulse, a concept which is central to our classical and semi-classical discussions in section 3.

Although the Kasevich–Chu interferometer has been discussed extensively in the literature we have not been able to find the analysis presented in this appendix. Moreover, the material is crucial for the understanding of the article and therefore keeps it self-contained.

#### A.1. Atom-laser interaction

We consider the center-of-mass motion of a three-level atom described [61] by the atomic Hamiltonian

$$\hat{H}_{a} \equiv \hbar \omega_{1} |g_{1}\rangle \langle g_{1}| + \hbar \omega_{2} |g_{2}\rangle \langle g_{2}| + \hbar \omega_{e} |e\rangle \langle e| \tag{A.1}$$

and shown in figure 1 as influenced by the interaction with the electromagnetic field

$$E(t) \equiv \mathcal{E}_1(t) e^{-i\nu_1 t} e^{i[k_1 z + \phi_1(t)]} + \mathcal{E}_2(t) e^{-i\nu_2 t} e^{-i[k_2 z + \phi_2(t)]}, \tag{A.2}$$

which consists of two counter-propagating waves of envelope  $\mathcal{E}_j = \mathcal{E}_j(t)$ , frequency  $\nu_j$ , wave vector  $k_j$  and phase  $\phi_j = \phi_j(t)$  where j = 1 and 2. Throughout our article we assume that the pulses are so short that the position of the atom is not influenced by it during its duration. Consequently, we for the time being neglect the dynamics of the center-of-mass motion of the atom and only take into account the interaction Hamiltonian

$$\hat{H}_{I} \equiv \hbar \Omega_{1}(t) |e\rangle \langle g_{1}| e^{-i\nu_{1}t} e^{i[k_{1}z + \phi_{1}(t)]} + \hbar \Omega_{2}(t) |e\rangle \langle g_{2}| e^{-i\nu_{2}t} e^{-i[k_{2}z + \phi_{2}(t)]} + \text{h.c.}$$
(A.3)

Here, the time-dependent Rabi frequencies  $\Omega_j = \Omega_j(t)$  involve the dipole moments of the transitions and the envelopes  $\mathcal{E}_j$  of the pulses. Moreover, the two different signs in the phases of the field reflect the fact that we deal with counter-propagating electromagnetic fields.

In the interaction picture defined by the atomic Hamiltonian  $\hat{H}_a$  the interaction Hamiltonian  $\hat{H}_{\rm I}^{({\rm I})} \equiv \exp(\mathrm{i}\hat{H}_a t/\hbar)\hat{H}_{\rm I} \exp(-\mathrm{i}\hat{H}_a t/\hbar)$  reads

$$\hat{H}_{\rm I}^{({\rm I})} \equiv \hbar \Omega_1(t) |e\rangle \langle g_1| e^{-i\Delta_1 t} e^{i[k_1 z + \phi_1(t)]} + \hbar \Omega_2(t) |e\rangle \langle g_2| e^{-i\Delta_2 t} e^{-i[k_2 z + \phi_2(t)]} + \text{h.c.}, \tag{A.4}$$

where we have introduced the detunings

$$\Delta_1 \equiv \nu_1 - (\omega_e - \omega_1) \tag{A.5}$$

and

$$\Delta_2 \equiv \nu_2 - (\omega_e - \omega_2) \tag{A.6}$$

between the two laser frequencies  $v_1$  and  $v_2$  and the frequencies  $\omega_e - \omega_1$  and  $\omega_e - \omega_2$  of the atomic transitions between  $|g_1\rangle$  and  $|e\rangle$  and  $|g_2\rangle$  and  $|e\rangle$ .

#### A.2. Quantum state of atom in perturbation theory

In the limit of large detunings  $\Delta_1$  and  $\Delta_2$  the interaction Hamiltonian  $\hat{H}_{\rm I}^{\rm (I)}$  oscillates rapidly. We gain insight into the resulting dynamics by the elementary perturbative expansion

$$|\psi_{\mathbf{a}}(t)\rangle \cong \left[\mathbb{1} - \frac{\mathrm{i}}{\hbar} \int_{0}^{t} \mathrm{d}t' \, \hat{H}_{\mathbf{I}}^{(\mathbf{I})}(t') - \frac{1}{\hbar^{2}} \int_{0}^{t} \mathrm{d}t' \int_{0}^{t'} \mathrm{d}t'' \, \hat{H}_{\mathbf{I}}^{(\mathbf{I})}(t') \hat{H}_{\mathbf{I}}^{(\mathbf{I})}(t'') \right] |\psi_{\mathbf{a}}(0)\rangle \tag{A.7}$$

of the time evolution of an initial atomic state  $|\psi_{\rm a}(0)
angle$  due to the Schrödinger equation with  $\hat{H}_{\rm I}^{({
m I})}$ .

A.2.1. Average of oscillatory terms. We first cast  $\hat{H}_{\rm I}^{\rm (I)}$  into the compact form

$$\hat{H}_{I}^{(I)} = \hat{A}_{1}(t)e^{-i\Delta_{1}t} + \hat{A}_{2}(t)e^{-i\Delta_{2}t} + \hat{A}_{1}^{\dagger}(t)e^{i\Delta_{1}t} + \hat{A}_{2}^{\dagger}(t)e^{i\Delta_{2}t}, \tag{A.8}$$

where the operators

$$\hat{A}_1(t) \equiv \hbar \Omega_1(t) \,e^{i[k_1 z + \phi_1(t)]} |e\rangle\langle g_1| \tag{A.9}$$

and

$$\hat{A}_2(t) \equiv \hbar \Omega_2(t) \,\mathrm{e}^{-\mathrm{i}[k_2 z + \phi_2(t)]} |e\rangle \langle g_2| \tag{A.10}$$

are slowly varying compared to their phase factors with the detunings  $\Delta_1$  and  $\Delta_2$ .

Hence, in the integration of  $\hat{H}_{\rm I}^{({\rm I})}$  over time we only integrate the phase factors, that is

$$\int_{0}^{t} dt' \, \hat{H}_{1}^{(I)}(t') = -\frac{\hat{A}_{1}(t)}{i\Delta_{1}} \left( e^{-i\Delta_{1}t} - 1 \right) - \frac{\hat{A}_{2}(t)}{i\Delta_{2}} \left( e^{-i\Delta_{2}t} - 1 \right) 
+ \frac{\hat{A}_{1}^{\dagger}(t)}{i\Delta_{1}} \left( e^{i\Delta_{1}t} - 1 \right) + \frac{\hat{A}_{2}^{\dagger}(t)}{i\Delta_{2}} \left( e^{i\Delta_{2}t} - 1 \right).$$
(A.11)

When we now average this result over the rapid oscillations due to  $\Delta_1$  and  $\Delta_2$  we arrive at

$$\overline{\int_0^t dt' \, \hat{H}_{\mathrm{I}}^{(\mathrm{I})}(t')} \cong \frac{\hat{A}_1(t)}{\mathrm{i}\Delta_1} + \frac{\hat{A}_2(t)}{\mathrm{i}\Delta_2} - \frac{\hat{A}_1^{\dagger}(t)}{\mathrm{i}\Delta_1} - \frac{\hat{A}_2^{\dagger}(t)}{\mathrm{i}\Delta_2}.$$
(A.12)

Here the bar indicates average over rapidly-oscillating terms.

As a result, in first order perturbation theory the time evolution of  $|\psi_a\rangle$  is governed by the slowly varying operators  $\hat{A}_j$  and  $\hat{A}_j^{\dagger}$  divided by the large detunings  $\Delta_j$ .

Next we turn to the second order perturbation theory which involves the product of  $\hat{H}_{\rm I}^{({\rm I})}(t)$  and the integral of  $\hat{H}_{\rm I}^{({\rm I})}$  given by (A.8) and (A.11). We only retain slowly varying terms, that is phase factors which contain the difference  $\Delta_- \equiv \Delta_1 - \Delta_2$  between the detunings. Phase factors which oscillate with  $\Delta_1$ ,  $\Delta_2$  or  $2\Delta_1$ ,  $2\Delta_2$  or  $\Delta_1 + \Delta_2$  we neglect since they will only provide small contributions in the integration over t'. As a result we find from (A.8) and (A.11) the formula

$$\hat{H}_{I}^{(I)}(t') \int_{0}^{t'} dt'' \, \hat{H}_{I}^{(I)}(t'') = \frac{\hat{A}_{1}\hat{A}_{1}^{\dagger}}{i\Delta_{1}} + \frac{\hat{A}_{1}\hat{A}_{2}^{\dagger}}{i\Delta_{2}} e^{-i\Delta_{-}t'} + \frac{\hat{A}_{2}\hat{A}_{1}^{\dagger}}{i\Delta_{1}} e^{i\Delta_{-}t'} + \frac{\hat{A}_{2}\hat{A}_{2}^{\dagger}}{i\Delta_{2}} - \frac{\hat{A}_{1}^{\dagger}\hat{A}_{1}}{i\Delta_{1}} - \frac{\hat{A}_{1}^{\dagger}\hat{A}_{2}}{i\Delta_{2}} e^{i\Delta_{-}t'} - \frac{\hat{A}_{2}^{\dagger}\hat{A}_{1}}{i\Delta_{1}} e^{-i\Delta_{-}t'} - \frac{\hat{A}_{2}^{\dagger}\hat{A}_{2}}{i\Delta_{2}}.$$
(A.13)

A.2.2. Explicit form of second order correction. We now evaluate the operator products and obtain from the definitions (A.9) and (A.10) the expressions

$$\hat{A}_1 \hat{A}_1^{\dagger} = \hbar^2 |\Omega_1|^2 |e\rangle \langle e| \tag{A.14}$$

and

$$\hat{A}_2 \hat{A}_2^{\dagger} = \hbar^2 |\Omega_2|^2 |e\rangle \langle e| \tag{A.15}$$

together with

$$\hat{A}_1^{\dagger} \hat{A}_1 = \hbar^2 |\Omega_1|^2 |g_1\rangle \langle g_1| \tag{A.16}$$

and

$$\hat{A}_{2}^{\dagger}\hat{A}_{2} = \hbar^{2}|\Omega_{2}|^{2}|g_{2}\rangle\langle g_{2}|. \tag{A.17}$$

Here we have assumed that the atomic states  $|g_1\rangle$ ,  $|g_2\rangle$  and  $|e\rangle$  are normalized.

Since  $|g_1\rangle$  and  $|g_2\rangle$  are orthogonal we obtain the identities

$$\hat{A}_1 \hat{A}_2^{\dagger} = 0 \tag{A.18}$$

and

$$\hat{A}_2 \hat{A}_1^{\dagger} = 0. \tag{A.19}$$

However, most important for our discussion of the interferometer are the products

$$\hat{A}_{1}^{\dagger}\hat{A}_{2} = \hbar^{2}\Omega_{1}^{*}\Omega_{2} e^{-i[kz+\phi_{+}(t)]}|g_{1}\rangle\langle g_{2}|$$
(A.20)

and

$$\hat{A}_{2}^{\dagger}\hat{A}_{1} = \hbar^{2}\Omega_{2}^{*}\Omega_{1} e^{i[kz+\phi_{+}(t)]}|g_{2}\rangle\langle g_{1}|, \tag{A.21}$$

where we have introduced the abbreviations

$$k \equiv k_1 + k_2 \tag{A.22}$$

and

$$\phi_{+} \equiv \phi_1 + \phi_2. \tag{A.23}$$

As a consequence, (A.13) reduces to

$$\int_{0}^{t'} dt'' \, \hat{H}_{1}^{(I)}(t') \, \hat{H}_{1}^{(I)}(t'') = \hbar^{2} \left( \frac{|\Omega_{1}|^{2}}{i\Delta_{1}} + \frac{|\Omega_{2}|^{2}}{i\Delta_{2}} \right) |e\rangle \langle e| - \hbar^{2} \frac{|\Omega_{1}|^{2}}{i\Delta_{1}} |g_{1}\rangle \langle g_{1}| 
- \hbar^{2} \frac{|\Omega_{2}|^{2}}{i\Delta_{2}} |g_{2}\rangle \langle g_{2}| - \hbar^{2} \frac{\Omega_{1}^{*}\Omega_{2}}{i\Delta_{2}} e^{-i(kz+\phi_{+})} e^{i\Delta_{-}t'} |g_{1}\rangle \langle g_{2}| 
- \hbar^{2} \frac{\Omega_{1}\Omega_{2}^{*}}{i\Delta_{1}} e^{i(kz+\phi_{+})} e^{-i\Delta_{-}t'} |g_{2}\rangle \langle g_{1}|,$$
(A.24)

which contains slowly-varying terms that are diagonal in the atomic states, and off-diagonal ones that oscillate with the difference  $\Delta_{-}$  of the two detunings. The diagonal ones cause an intensity-dependent shift of the atomic levels. Since the main interest of this appendix is the description of the Kasevich-Chu interferometer we do not discuss these shifts further but solely focus on the terms that cause a transition from  $|g_1\rangle$  to  $|g_2\rangle$  and back.

A.2.3. State after pulse for identical detunings. The special choice of identical detunings, that is  $\Delta_{-} = 0$  and neglecting the intensity-dependent shifts leads us to the expression

$$\int_{0}^{t'} dt'' \, \hat{H}_{I}^{(I)}(t') \, \hat{H}_{I}^{(I)}(t'') = i\hbar^{2} \left[ \Omega(t) e^{i(kz+\phi_{+})} \, \hat{\sigma}^{\dagger} + \Omega^{*}(t) e^{-i(kz+\phi_{+})} \, \hat{\sigma} \right], \tag{A.25}$$

where we have introduced the abbreviation

$$\Omega(t) \equiv \frac{\Omega_1(t)\Omega_2^*(t)}{\nu_1 - (\omega_e - \omega_1)} = \frac{\Omega_1(t)\Omega_2^*(t)}{\nu_2 - (\omega_e - \omega_2)}$$
(A.26)

and the Pauli spin matrices  $\hat{\sigma}^{\dagger} \equiv |g_2\rangle\langle g_1|$  and  $\hat{\sigma} \equiv |g_1\rangle\langle g_2|$  for the transition from  $|g_1\rangle$  to  $|g_2\rangle$  and from  $|g_2\rangle$  to  $|g_1\rangle$ , respectively. Moreover, we have taken advantage in (A.26) of the fact that  $\Delta_1 = \Delta_2$ .

We are now in the position to obtain the final expression for the quantum state  $|\psi_a\rangle$  in second order perturbation. Here we integrate over the full duration of the laser pulse, which is assumed to be symmetric around t=0, that is we integrate from  $-\infty$  to  $+\infty$ . Moreover, we neglect the contribution (A.12) from first order perturbation theory compared to the second order since it only involves slowly varying terms compared to the *integral* of slowly varying terms.

When we substitute (A.25) into (A.7) we find

$$|\psi_{\mathbf{a}}(+\infty)\rangle \cong \left[\mathbb{1} - \mathrm{i}\left(\theta \,\mathrm{e}^{\mathrm{i}\varphi}\hat{\sigma}^{\dagger} + \theta \,\mathrm{e}^{-\mathrm{i}\varphi}\hat{\sigma}\right)\right]|\psi_{\mathbf{a}}(-\infty)\rangle,$$
 (A.27)

where we have introduced the abbreviation

$$\int_{-\infty}^{\infty} dt \ \Omega(t) \equiv \theta \ e^{i\beta_{\Omega}}, \tag{A.28}$$

which involves the real-valued pulse area  $\theta$  and a phase  $\beta_{\Omega}$  which emerges from the fact that the product  $\Omega_1\Omega_2^*$  of the two Rabi frequencies may be complex.

The total phase

$$\varphi \equiv kz + \phi(0) \tag{A.29}$$

contains the position z of the atom in the superposition of the two counterpropagating waves of total wave vector  $k \equiv k_1 + k_2$  and the sum

$$\phi \equiv \beta_{\Omega} + \phi_{+} = \beta_{\Omega} + \phi_{1} + \phi_{2} \tag{A.30}$$

of the phase  $\beta_{\Omega}$  of the complex-valued pulse area and the sum  $\phi_{+} \equiv \phi_{1} + \phi_{2}$  of the phases of the two waves. For simplicity we evaluate  $\phi$  at the center of the pulse, that is at t = 0.

In view of perturbation theory we can also interpret the correction to the identity operator in (A.27) as the first term of the power expansion of an exponential and obtain the approximate relation

$$|\psi_a(+\infty)\rangle \cong \hat{U}_1|\psi_a(-\infty)\rangle,$$
 (A.31)

where the unitary operator

$$\hat{U}_{\rm I} \equiv \exp[-i(\theta \, e^{i\varphi} \hat{\sigma}^{\dagger} + \theta \, e^{-i\varphi} \hat{\sigma})] \tag{A.32}$$

connects  $|\psi_a(-\infty)\rangle$  with  $|\psi_a(+\infty)\rangle$ .

A.2.4. Summary. Due to the large detunings  $\Delta_1$  and  $\Delta_2$  we have been able to eliminate the excited state  $|e\rangle$  and we deal only with a two-level atom with states  $|g_1\rangle$  and  $|g_2\rangle$  driven by an electromagnetic field whose time dependence originates from the envelopes  $\mathcal{E}_1$  and  $\mathcal{E}_2$  of the two pulses and is therefore slow compared to optical frequencies. Hence, the internal dynamics of the atom for a short pulse at t=0 is governed by the unitary operator  $\hat{U}_1$  defined by (A.32).

#### A.3. Analysis of the unitary operator

We now evaluate  $\hat{U}_{\rm I}$  and find from the identity [61]

$$\exp\left[-i(\theta e^{i\varphi}\hat{\sigma}^{\dagger} + \theta e^{-i\varphi}\hat{\sigma})\right] = \cos\theta - i\sin\theta \left[e^{i\varphi}\hat{\sigma}^{\dagger} + e^{-i\varphi}\hat{\sigma}\right]$$
(A.33)

familiar from the Jaynes–Cummings model and from (A.29) the representation

$$\hat{U}_{I} = \cos \theta - i \sin \theta \left[ e^{i(kz + \phi(0))} |g_{2}\rangle\langle g_{1}| + e^{-i(kz + \phi(0))} |g_{1}\rangle\langle g_{2}| \right]$$
(A.34)

of the internal dynamics due to the laser pulse.

Indeed, when we start from a given atomic state we can either remain in it with the probability amplitude  $\cos\theta$  determined by the pulse area  $\theta$ , or we make a transition with a probability amplitude  $(-i\sin\theta)$ . In the latter case the initial state is of importance. Indeed, when we start from  $|g_1\rangle$  and make a transition to  $|g_2\rangle$ , that is we absorb a photon from the laser pulse, we have to multiply the state by the phase factor  $\exp[i(kz+\phi(0))]$ . In contrast, when we begin in the state  $|g_2\rangle$  and end up in  $|g_1\rangle$ , that is we emit a photon, we multiply by the phase factor  $\exp[-i(kz+\phi(0))]$ .

The terms  $\cos\theta$  and  $(-i\sin\theta)$  ensure the unitarity condition

$$\hat{U}_{\mathbf{I}}\hat{U}_{\mathbf{I}}^{\dagger} = \hat{U}_{\mathbf{I}}^{\dagger}\hat{U}_{\mathbf{I}} = \mathbb{1}. \tag{A.35}$$

Indeed, we find from (A.34) in the form

$$\hat{U}_{I} = \cos \theta - i \sin \theta [e^{i\varphi} \hat{\sigma}^{\dagger} + e^{-i\varphi} \hat{\sigma}]$$
(A.36)

and

$$\hat{U}_{\rm I}^{\dagger} = \cos\theta + i\sin\theta \left[ e^{-i\varphi}\hat{\sigma} + e^{i\varphi}\hat{\sigma}^{\dagger} \right] \tag{A.37}$$

the relation

$$\hat{U}_{\mathbf{I}}\hat{U}_{\mathbf{I}}^{\dagger} = \cos^2\theta + \sin^2\theta [\hat{\sigma}^{\dagger}\hat{\sigma} + e^{2i\varphi}\hat{\sigma}^{\dagger^2} + e^{-2i\varphi}\hat{\sigma}^2 + \hat{\sigma}\hat{\sigma}^{\dagger}], \tag{A.38}$$

which with the properties

$$\hat{\sigma}^2 = \hat{\sigma}^{\dagger 2} = 0$$
 and  $\hat{\sigma}\hat{\sigma}^{\dagger} + \hat{\sigma}^{\dagger}\hat{\sigma} = \mathbb{1}$  (A.39)

of the Pauli matrices  $\hat{\sigma}$  and  $\hat{\sigma}^{\dagger}$  leads us to (A.35).

### A.4. Beam splitters and mirrors

On first sight the position-dependent phase factor in (A.34) does not seem to be important. However, when we also describe the center-of-mass motion of the atom quantum mechanically the coordinate z of the atom turns into an operator  $\hat{z}$  and we finally arrive at the unitary operators

$$\hat{U}^{(\pm)}(t) \equiv e^{\pm i[k\hat{z} + \phi(t)]} \tag{A.40}$$

acting on the initial quantum state  $|\psi_i\rangle$  of the center-of-mass motion. Here the plus or the minus sign correspond to the transitions from  $|g_1\rangle$  to  $|g_2\rangle$  or from  $|g_2\rangle$  to  $|g_1\rangle$ , respectively.

We note that by an appropriate choice of the pulse envelopes  $\mathcal{E}_1$  and  $\mathcal{E}_2$  determining by (A.26) and (A.28) the pulse area  $\theta$  we can even create a 50:50 beam splitter, or a mirror. Indeed, when we choose  $\theta = \pi/4$  we find with  $\cos(\pi/4) = \sin(\pi/4) = 1/\sqrt{2}$  a coherent superposition of two states of the center-of-mass motion since we superpose with equal probability amplitudes the initial  $|\psi_i\rangle$  state with  $\hat{U}^{(\pm)}|\psi_i\rangle$ . Hence, we have realized a beam splitter for atoms. Moreover, we note from (A.34) that the state of the deflected atom has to be multiplied by (-i).

On the other hand the choice  $\theta = \pi/2$  with  $\cos(\pi/2) = 0$  eliminates the possibility to remain in the state and we always change  $|\psi_i\rangle$ . Although there is no new superposition formed

by this interaction the center-of-mass motion is dramatically influenced by the unitary operators  $\hat{U}^{(\pm)}$  acting on  $|\psi_i\rangle$ . Indeed, the atom is deflected similarly to light by a mirror. Hence, this choice of the laser parameters corresponds to a mirror for atoms. Again the quantum state has to be multiplied by (-i) as indicated by (A.34).

We conclude by briefly discussing the Kasevich–Chu interferometer shown in figure 1. Here the three laser pulses are chosen such that the first and the third one serve as 50:50 beam splitters with  $\cos(\pi/4) = \sin(\pi/4) = 1/\sqrt{2}$  while the second one is a mirror with  $\cos(\pi/2) = 0$ . As a result, every beam splitter brings in a factor  $1/\sqrt{2}$  for the two interfering quantum states.

# A.5. Effective potential corresponding to laser pulse

In the preceding section we have obtained the expression (A.40) for the unitary transformations  $\hat{U}^{(+)}$  and  $\hat{U}^{(-)}$  associated with a transition from the atomic state  $|g_1\rangle$  to  $|g_2\rangle$  and from  $|g_2\rangle$  to  $|g_1\rangle$ , respectively. We now show that we can interpret  $\hat{U}^{(\pm)}$  as the result of the unitary time evolution due to the Hamiltonian

$$\hat{H}_{lp} \equiv \frac{\hat{p}^2}{2m} + V_{lp}(\hat{z}, t)$$
 (A.41)

with the effective time- and position-dependent potential

$$V_{\rm lp}(\hat{z},t) \equiv \mp \hbar \left[ k \hat{z} + \phi(T) \right] \delta(t-T). \tag{A.42}$$

Here we have approximated the short laser pulse acting at t = T by a delta function.

During the duration of the pulse we can neglect the kinetic energy compared to  $V_{\rm lp}$ , and the quantum state  $|\psi(T+\delta)\rangle$  of the center-of-mass motion, shortly after the pulse, is connected to the state  $|\psi(T-\delta)\rangle$  shortly before the pulse by the solution of the corresponding Schrödinger equation

$$i\hbar \frac{\mathrm{d}}{\mathrm{d}t} |\psi(t)\rangle = \hat{H}_{\mathrm{lp}} |\psi(t)\rangle \cong V_{\mathrm{lp}}(t) |\psi(t)\rangle$$
 (A.43)

which reads

$$|\psi(T+\delta)\rangle = \exp\left[-\frac{\mathrm{i}}{\hbar} \int_{T-\delta}^{T+\delta} \mathrm{d}t \ V_{\mathrm{lp}}(t)\right] |\psi(T-\delta)\rangle.$$
 (A.44)

With the help of the definition (A.42) of  $V_{lp}$  we find immediately

$$|\psi(T+\delta)\rangle = \exp\{\pm i \left[k\hat{z} + \phi(T)\right]\} |\psi(T-\delta)\rangle = \hat{U}^{(\pm)}(T)|\psi(T-\delta)\rangle. \quad (A.45)$$

Hence, we can describe in the case of an internal transition the action of a laser pulse on the center-of-mass motion of the atom by the effective potential  $V_{\rm lp}$ . In particular, the excitation of the atom from  $|g_1\rangle$  to  $|g_2\rangle$  requires the minus sign in  $V_{\rm lp}$  whereas the deexcitation from  $|g_2\rangle$  to  $|g_1\rangle$  is associated with the plus sign. In section 3 we show using  $V_{\rm lp}$  and classical mechanics that these processes give rise to an increase, or a decrease of the momentum of the atom by  $\hbar k$ . Needless to say, this statement also holds true when we describe the motion by quantum mechanics as discussed in section 6. In case the atom is unaffected by the laser pulse and remains in its internal state the potential  $V_{\rm lp}$  vanishes and no momentum transfer occurs.

### Appendix B. Semi-classical considerations in phase space

Sections 2 and 3 of our article are based on the assumption that the phase of the wave function is given by the action of the atom evaluated along its classical trajectory. In order to give credence to this assumption we connect in this appendix the Lagrangian with the Hamiltonian formulation of quantum mechanics in the semi-classical limit, and obtain in this way the phase of the energy wave function in the WKB-approximation. Moreover, we present the resolution of a riddle put forward in [60] where we had found that the area in phase space circumvented by the atom is *twice* the phase shift due to the acceleration. We identify the origin of this factor and rederive the total phase shift in the interferometer.

## B.1. Connection to WKB-wave function

We start by connecting the Lagrange formalism with the WKB-expression of an energy wave function. For this purpose we first cast the action due to the Lagrangian

$$\mathcal{L} \equiv \frac{1}{2}mv^2 - V(z, t) \tag{B.1}$$

with a space- and time-dependent potential V in terms of the Hamiltonian

$$H \equiv \frac{p^2}{2m} + V(z, t). \tag{B.2}$$

For a potential V that is independent of  $v \equiv \dot{z}$  we find with the help of the Legendre transformation

$$\mathcal{L} = \dot{z}p - H \tag{B.3}$$

the connection formula

$$\int dt \, \mathcal{L} = \int dz \, p - \int dt \, H \tag{B.4}$$

and we can derive from the non-relativistic limit of the de Broglie wave (7) neglecting the contribution  $mc^2t/\hbar$ , that is, from

$$\psi = \exp\left(\frac{i}{\hbar} \int dt \,\mathcal{L}\right) \tag{B.5}$$

the expression

$$\psi \equiv e^{i\beta} \equiv \exp\left(-\frac{i}{\hbar} \int dt \ H\right) \exp\left(\frac{i}{\hbar} \int dz \ p\right)$$
 (B.6)

for a wave function in terms of the classical Hamiltonian H and momentum p. We emphasize that here we have focused only on the phase and not on the amplitude of  $\psi$ .

For a time-independent Hamiltonian, that is for  $H \equiv E$ , (B.6) reduces to

$$\psi = \exp\left(-\frac{\mathrm{i}}{\hbar}Et\right) \exp\left(\frac{\mathrm{i}}{\hbar} \int_{z_0}^z \mathrm{d}\tilde{z} \, p\right) \tag{B.7}$$

familiar from the WKB-representation [61] of an energy wave function.

**Table B.1.** Evaluation of dynamical phase in the Kasevich–Chu atom interferometer associated with the Hamiltonian  $H_g$  consisting solely of kinetic and gravitational energies. Due to the momentum transfer from the laser pulses the energy is not conserved during the complete motion of the atom through the interferometer. However, between the pulses there is conservation of energy which allows us to evaluate the dynamical phase in an efficient way. We emphasize that this phase only includes the dynamical effects arising from the gravitational field but not from the interaction of the laser pulses with the atom. The position  $z_g(2T)$  and velocity  $v_g(2T)$  of the atom in the linear gravitational field  $V_g$  shortly after the third laser pulse read  $z_g(2T) \equiv z_g(0) + v_g(0)2T - 2gT^2$  and  $v_g(2T) \equiv v_g(0) - 2gT$  where  $z_g(0)$  and  $v_g(0)$  denote the position and velocity shortly before the first pulse.

	Between 0 and T	Between T and 2T
Energy $E_{\rm u}$ on upper path	$\frac{1}{2}m[v_g(0) + \frac{\hbar k}{m}]^2 + V_g(z_g(0))$	$\frac{1}{2}m  v_g(2T)^2 + V_g(z_g(2T))$
Energy $E_1$ on lower path Difference	$\frac{1}{2}m[v_g(0)]^2 + V_g(z_g(0))$	$\frac{1}{2}m[v_g(2T) + \frac{\hbar k}{m}]^2 + V_g(z_g(2T))$
$E_{-} \equiv E_{\rm u} - E_{\rm l}$ of energies	$\frac{1}{2}m[2v_g(0)\tfrac{\hbar k}{m}+(\tfrac{\hbar k}{m})^2]$	$-\tfrac{1}{2}m[2v_g(2T)\tfrac{\hbar k}{m}+(\tfrac{\hbar k}{m})^2]$
$\frac{1}{\hbar} \oint \mathrm{d}t \ H_g$	$k[v_g(0) - v_g(2T)]T = -2k\ddot{z}_g(0)T^2 = 2k gT^2 = 2\delta\varphi_g$	

### B.2. Resolution of a small puzzle

Recently the authors of [60] have made the puzzling observation that the area in phase space circumvented by the closed classical trajectory of an atom in the Kasevich–Chu interferometer when expressed in units of  $\hbar$  is *twice* the phase shift due to the acceleration of the atom. The well-known identity

$$\oint dz \, p = 2 \oint dt \, \left(\frac{1}{2} m v^2\right) \tag{B.8}$$

states that this area is twice the action due to the kinetic energy which according to table 1 is given by  $\hbar\delta\varphi_g$ . Hence, we arrive at the relation

$$\frac{1}{\hbar} \oint dz \, p = 2\delta \varphi_g, \tag{B.9}$$

that is, the area in phase space in units of  $\hbar$  is indeed  $2\delta\varphi_g$ , which confirms and explains the claim of [60].

Since according to (32) the action given by  $\mathcal{L}_g$  along the closed classical trajectory determined by  $\mathcal{L}$  vanishes the connection formula (B.4) together with (B.9) predicts

$$\frac{1}{\hbar} \oint dt \, H_g = 2\delta \varphi_g \tag{B.10}$$

which is again *twice*  $\delta \varphi_g$ . In table B.1 we verify that this claim is indeed correct.

One might therefore wonder: what is the origin of the phase shift  $\alpha$  in this phase space picture? The answer to this question springs from the considerations of section 3. Indeed, the dynamics of the system does not result from  $H_g$  but from  $H = H_g + V_{lp}$  which apart from the gravitational potential  $V_g$  also contains the potential energy  $V_{lp}$  due to the laser pulses. Thus we find from (B.6) for the phase  $\beta$  of the matter wave after a completion of the path the expression

$$\beta \equiv -\frac{1}{\hbar} \oint dt \ H + \frac{1}{\hbar} \oint dz \ p = -\frac{1}{\hbar} \oint dt \ H_g - \frac{1}{\hbar} \oint dt \ V_{lp} + \frac{1}{\hbar} \oint dz \ p \qquad (B.11)$$

which reduces with (B.9), (B.10) and (25) to

$$\beta = -2\delta\varphi_{\varrho} + \alpha + 2\delta\varphi_{\varrho} = \alpha, \tag{B.12}$$

in complete agreement with our previous analysis.

### Appendix C. Operator identity

In this appendix we rederive for the sake of completeness the relation

$$\hat{U} \equiv e^{-ik\hat{z}} e^{-i\hat{H}T/\hbar} e^{ik\hat{z}} = e^{-i\hat{H}^{(+)}T/\hbar}, \tag{C.1}$$

where

$$\hat{H} \equiv \frac{\hat{p}^2}{2m} + V(\hat{z}) \tag{C.2}$$

and

$$\hat{H}^{(+)} \equiv \frac{(\hat{p} + \hbar k)^2}{2m} + V(\hat{z}). \tag{C.3}$$

Here we slightly generalize the derivation of [60]. Indeed the present treatment holds true for any potential V = V(z) that only depends on z.

For this purpose we first expand the exponential with  $\hat{H}$  into a power series and insert the unity operator  $\mathbb 1$  in the form

$$e^{ik\hat{z}} e^{-ik\hat{z}} \equiv 1 \tag{C.4}$$

between the individual terms of  $\hat{H}^n$  which yields

$$\hat{U} = \sum_{n=0}^{\infty} \frac{1}{n!} \left( \frac{-iT}{\hbar} \right)^n \left( e^{-ik\hat{z}} \hat{H} e^{ik\hat{z}} \right) \left( e^{-ik\hat{z}} \hat{H} e^{ik\hat{z}} \right) \dots \left( e^{-ik\hat{z}} \hat{H} e^{ik\hat{z}} \right). \tag{C.5}$$

Moreover, we note the identity

$$e^{-ik\hat{z}} \hat{p}^2 e^{ik\hat{z}} = (\hat{p} + \hbar k)^2$$
 (C.6)

and find

$$e^{-ik\hat{z}} \hat{H} e^{ik\hat{z}} = e^{-ik\hat{z}} \left( \frac{\hat{p}^2}{2m} + V(\hat{z}) \right) e^{ik\hat{z}} = \frac{(\hat{p} + \hbar k)^2}{2m} + V(\hat{z}) = \hat{H}^{(+)},$$
 (C.7)

which together with equation (C.5) leads to the desired result equation (C.1).

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## Appendix D. Time evolution of a momentum state in a linear potential

In this appendix we study the propagation of a momentum eigenstate  $|p\rangle$  in a linear potential  $V(z) \equiv \gamma z$  of steepness  $\gamma$  given by the Hamiltonian

$$\hat{H}_1 \equiv \frac{\hat{p}^2}{2m} + \gamma \hat{z}.\tag{D.1}$$

We show by taking advantage of the completeness relations of the energy and momentum eigenstates  $|E\rangle$  and  $|p'\rangle$ , respectively and the momentum representation of  $|E\rangle$  that a momentum eigenstate remains a momentum eigenstate but acquires a phase. For a different derivation we refer to the lectures [63] of Cohen-Tannoudji at the Collège de France. We conclude by deriving two alternative but completely equivalent representations of this phase factor and illustrate our result with the help of the Wigner function formulation [61] of quantum mechanics.

### D.1. Derivation

The completeness relations of the energy eigenstates  $|E\rangle$  defined by  $\hat{H}_1|E\rangle = E|E\rangle$  and the momentum eigenstates  $|p'\rangle$  given by  $\hat{p}|p\rangle = p|p\rangle$  provide us with the identity

$$\exp\left(-\frac{\mathrm{i}}{\hbar}\hat{H}_{1}t\right)|p\rangle = \int_{-\infty}^{\infty} \mathrm{d}E \int_{-\infty}^{\infty} \mathrm{d}p' \,\mathrm{e}^{-\mathrm{i}Et/\hbar}u_{E}^{*}(p)u_{E}(p')|p'\rangle,\tag{D.2}$$

where the momentum representation  $u_E(p) \equiv \langle p|E \rangle$  of  $|E\rangle$  follows from the eigenvalue equation

$$\left(\frac{p^2}{2m} - \gamma \frac{\hbar}{i} \frac{d}{dp}\right) u_E(p) = E u_E(p)$$
(D.3)

of  $|E\rangle$  in momentum space. Direct integration of this differential equation of first order in p yields

$$u_E(p) = \mathcal{N}\exp\left[\frac{\mathrm{i}}{\hbar\nu}\left(\frac{p^3}{6m} - Ep\right)\right],\tag{D.4}$$

where the normalization constant N is determined by the condition

$$\int_{-\infty}^{\infty} dE \, u_E^*(p) \, u_E(p') = \delta(p - p'), \tag{D.5}$$

which with the explicit form (D.4) of  $u_E$  reads

$$|\mathcal{M}|^2 \int_{-\infty}^{\infty} dE \, \exp\left[i(p-p')\frac{E}{\hbar \gamma}\right] \exp\left[-\frac{i}{6\hbar \gamma m}(p^3-p'^3)\right] = \delta(p-p'). \quad (D.6)$$

The integral over E is a Dirac delta function provided

$$|\mathcal{M}|^2 = \frac{1}{2\pi\hbar\gamma},\tag{D.7}$$

in which case the difference of the cubes of momenta in the phase factor vanishes and we obtain the desired orthonormality (D.6).

When we now substitute the expressions (D.4) and (D.7) for  $u_E$  and  $|\mathcal{N}|^2$  into (D.2) we arrive at

$$\exp\left(-\frac{\mathrm{i}}{\hbar}\hat{H}_{1}t\right)|p\rangle = \int_{-\infty}^{\infty} \mathrm{d}p' \, \frac{1}{2\pi\hbar\gamma} \int_{-\infty}^{\infty} \mathrm{d}E \, \exp\left[-\mathrm{i}(\gamma t - p + p')\frac{E}{\hbar\gamma}\right] \tag{D.8}$$

$$\times \exp\left[-\frac{\mathrm{i}}{6\hbar\gamma m}(p^3 - p'^3)\right]|p'\rangle. \tag{D.9}$$

The integration over E yields a delta function in the variable  $\gamma t - p + p'$  which allows us to perform the integration over p' and we find the relation

$$\exp\left(-\frac{\mathrm{i}}{\hbar}\hat{H}_{1}t\right)|p(0)\rangle = \exp\left\{-\mathrm{i}\left[\kappa(p(0)) - \kappa(p(t))\right]\right\}|p(t)\rangle,\tag{D.10}$$

where

$$p(t) \equiv p(0) - \gamma t \tag{D.11}$$

is the time-dependent momentum given by the integration of the Newton equation  $\dot{p} = -\gamma$  for a linear potential and the phase

$$\kappa(p) \equiv \frac{1}{6\hbar\gamma m} p^3 \tag{D.12}$$

is cubic in the momentum.

## D.2. Alternative representation of phase factor

In (D.10) the phase factor is given by the difference between  $\kappa$  at the initial and the final momentum. Due to the form (D.11) of p(t) the terms cubic in p(0) cancel and the phase only involves terms quadratic in the initial momentum. Indeed, with the identity

$$a^{3} - (a - b)^{3} = 3b \left[ \left( a - \frac{1}{2}b \right)^{2} + \frac{1}{12}b^{2} \right],$$
 (D.13)

we can re-express the difference  $p(0)^3 - (p(0) - \gamma t)^3$  and find the alternative representation

$$\exp\left(-\frac{\mathrm{i}}{\hbar}\hat{H}_{1}t\right)|p(0)\rangle = \exp\left[-\frac{\mathrm{i}}{\hbar}\epsilon(p(0);t)t\right]|p(t)\rangle \tag{D.14}$$

of the time evolution of a momentum state in a linear potential where we have introduced the quantity

$$\epsilon(p(0);t) \equiv \frac{1}{2m} \left[ p(0) - \frac{1}{2}\gamma t \right]^2 + \frac{1}{24m} (\gamma t)^2.$$
 (D.15)

### D.3. Wigner function analysis

We conclude this appendix by noting that the result that in the time evolution a momentum state remains a momentum state is also confirmed in the Wigner function formulation [61] of quantum mechanics. Indeed, for a linear potential the dynamics of the Wigner function is determined [60, 61] by the classical Liouville equation, that is we follow classical trajectories. As a result the Wigner function

$$W(z, p; t) = W_0 \left( z - \frac{p}{m} t - \frac{1}{m} \gamma t^2; p + \gamma t \right)$$
 (D.16)

at time t is given in terms of the initial Wigner function  $W_0$  with re-scaled variables.

Since the Wigner function of a momentum eigenstate  $|p(0)\rangle$  is a Dirac delta function, that is

$$W_0(z, p) = \frac{1}{2\pi\hbar} \delta(p - p(0)), \tag{D.17}$$

the Wigner function at time t reads

$$W_0(z, p; t) = \frac{1}{2\pi\hbar} \delta(p - (p(0) - \gamma t)) = \frac{1}{2\pi\hbar} \delta(p - p(t))$$
 (D.18)

in complete agreement with equation (D.10). Unfortunately the Wigner function cannot provide us with the phase factor in (D.14) since it is bilinear in the wave function.

It is interesting to note that the Wigner function treatment already indicates that in contrast to the momentum eigenstate a position eigenstate  $|z\rangle$  cannot remain a position eigenstate under the time evolution in a linear potential. From the state vector formulation of quantum mechanics this fact is obvious since the matrix element  $\langle z''| \exp(-i\hat{H}_1t/\hbar)|z\rangle$  is the propagator G.

From the expression (D.16) for the time-evolved Wigner function of the initial Wigner function

$$W_0(z, p) = \frac{1}{2\pi\hbar} \delta(z - z(0))$$
 (D.19)

corresponding to the position eigenstate  $|z(0)\rangle$  we find

$$W(z, p; t) = \frac{1}{2\pi\hbar} \delta \left[ z - \left( z(0) + \frac{p}{m}t + \frac{1}{m}\gamma t^2 \right) \right].$$
 (D.20)

Although the expression in the round parentheses of the argument of the delta function is reminiscent of the time dependent position coordinate z(t) of a particle in a linear potential it cannot be interpreted as  $|z(t)\rangle$  since the conjugate variable p enters. Indeed, in the position representation of quantum mechanics momentum cannot appear.

### Appendix E. Integration over all paths by method of stationary phase

In section 7 we have evaluated the matrix element  $M \equiv \langle z'''|\hat{U}_1^{\dagger}\hat{U}_u|z\rangle$  determining the operator product  $\hat{U}_1^{\dagger}\hat{U}_u$  in position space, and given according to (118) by a triple integral, by performing first the integration over the common end point z'' of the two paths in the interferometer, and then the integrations over the mid points z' and  $\tilde{z}'$ . In the present section we follow a different route and first integrate over z' and  $\tilde{z}'$ , and then over z''. Since the integrals over z' and  $\tilde{z}'$  are independent of each other and only involve quadratic phase factors they can be calculated in a straightforward way. In particular, the method of stationary phase which in this case is exact,

allows us to make contact with the classical trajectories discussed in section 3. However, there is a subtlety: the path is not closed until we have completed the integration over z'' which creates a delta function and makes the matrix element  $M \equiv \langle z''' | \hat{U}_1^{\dagger} \hat{U}_u | z \rangle$  diagonal such that the initial and the final coordinates z and z''' are identical.

## E.1. Integration over mid point and emergence of two paths

We now evaluate the matrix element

$$M = e^{i\delta\phi} \frac{1}{2\pi} \frac{m}{2\hbar T} \int_{-\infty}^{\infty} dz'' I_1^*(z'', z''') I_u(z'', z), \tag{E.1}$$

where we have introduced the abbreviations

$$I_{\rm u}(z'',z) = \sqrt{\frac{m}{{\rm i}\pi\hbar T}} \int_{-\infty}^{\infty} {\rm d}z' \, \exp\left[\frac{{\rm i}}{\hbar} \Lambda_{\rm u}(z';z'',z)\right] \tag{E.2}$$

and

$$I_{1}(z'', z''') = \sqrt{\frac{m}{i\pi\hbar T}} \int_{-\infty}^{\infty} d\tilde{z}' \exp\left[\frac{i}{\hbar} \Lambda_{1}(\tilde{z}'; z'', z''')\right]. \tag{E.3}$$

Here we have recalled the definition (112) of N and the phases

$$\Lambda_{\rm u}(z'; z'', z) \equiv S_{\rm cl}(z'', T|z') + S_{\rm cl}(z', T|z) + \hbar k(-z' + z) \tag{E.4}$$

and

$$\Lambda_{l}(\tilde{z}'; z'', z''') \equiv S_{cl}(z'', T|\tilde{z}') + S_{cl}(\tilde{z}', T|z''') + \hbar k(-z'' + \tilde{z}')$$
(E.5)

accumulated on the upper and lower path contain the classical action

$$S_{cl}(z', T|z) \equiv \frac{m}{2T}(z'-z)^2 - \frac{1}{2}(z+z')mgT - \frac{1}{24}mg^2T^3.$$
 (E.6)

Since the integration variables z' and  $\tilde{z}'$  in (E.2) and (E.3) appear in the phases  $\Lambda_u$  and  $\Lambda_l$  by virtue of the classical action  $S_{cl}$  given by (E.6) at most quadratically we can perform these integrations with the help of the integral relation

$$\int_{-\infty}^{\infty} d\theta \, e^{i\gamma\theta^2} = \sqrt{\frac{i\pi}{\gamma}} \tag{E.7}$$

in an exact way.

However, it is more intuitive to evaluate the integrals using the method of stationary phase, which for phases quadratic in the integration variable is exact. The points  $z'_u$  and  $z'_l$  of stationary phase of  $\Lambda_u$  and  $\Lambda_l$  select from a continuum of trajectories on the upper and lower path a single one and follow from the conditions

$$0 = \frac{\partial \Lambda_{\mathbf{u}}}{\partial z'} \bigg|_{z'=z'_{\mathbf{u}}} = \left[ \frac{m}{T} (-z'' + 2z' - z) - mgT - \hbar k \right] \bigg|_{z'=z'_{\mathbf{u}}}$$
(E.8)

and

$$0 = \frac{\partial \Lambda_1}{\partial \tilde{z}'} \bigg|_{\tilde{z}' = z_1'} = \left[ \frac{m}{T} (-z'' + 2\tilde{z}' - z''') - mgT + \hbar k \right] \bigg|_{\tilde{z}' = z_1'}, \tag{E.9}$$

where we have recalled the definitions (E.4)–(E.6) of  $\Lambda_u$ ,  $\Lambda_1$  and  $S_{cl}$ , respectively.

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The points

$$z'_{\rm u} \equiv \frac{1}{2}(z'' + z) + \frac{\hbar k}{2m}T + \frac{1}{2}gT^2$$
 (E.10)

and

$$z'_{1} \equiv \frac{1}{2}(z'' + z''') - \frac{\hbar k}{2m}T + \frac{1}{2}gT^{2}$$
(E.11)

of stationary phase together with the expressions

$$\frac{\partial^2}{\partial z'^2} \Lambda_{\rm u} = \frac{2m}{T} \quad \text{and} \quad \frac{\partial^2}{\partial \tilde{z}'^2} \Lambda_{\rm l} = \frac{2m}{T}$$
 (E.12)

for the second derivatives following from (E.8) and (E.9) together with the integral relation (E.7) allow us to perform the integrations over z' and  $\tilde{z}'$  in (E.2) and (E.3) in an exact way and we find the expressions

$$I_{\rm u} = \exp\left[\frac{\mathrm{i}}{\hbar}\Lambda_{\rm u}(z'_{\rm u}; z'', z)\right] \tag{E.13}$$

and

$$I_{l} = \exp\left[\frac{\mathrm{i}}{\hbar}\Lambda_{l}(z_{l}'; z'', z''')\right]. \tag{E.14}$$

Hence, the method of stationary phase shows us how a single trajectory emerges from the interference of all possible paths. Indeed, from a continuum of mid points z' and  $\tilde{z}'$  only  $z'_u$  and  $z'_1$  defined by (E.10) and (E.11) are relevant. As a result we can interpret the motion of the atom as starting at z, and reaching z'' on the upper path via  $z'_u$ , whereas on the lower path it begins at z''' and arrives at z'' by going through  $z'_1$ . The phases accumulated during these motions are  $\Lambda_u(z'_u; z'', z)$  and  $\Lambda_1(z'_1; z'', z''')$  evaluated at the mid points  $z'_u$  and  $z'_1$ .

### E.2. Diagonal structure from interference of end points

However, it is important to note that so far we deal with two distinct start points z and z'''. Only when we integrate over z'' do we get the condition z = z''', that is a closed path.

In order to verify this claim we substitute (E.13) and (E.14) into equation (E.1) for the matrix element M and arrive at

$$M = e^{i\delta\phi} \frac{1}{2\pi} \frac{m}{2\hbar T} \int_{-\infty}^{\infty} dz'' \exp\left[\frac{i}{\hbar} \Lambda_{-}(z'')\right]$$
 (E.15)

where with the help of the definitions (E.4) and (E.5) the difference

$$\Lambda_{-}(z'') \equiv \Lambda_{11}(z'_{11}; z'', z) - \Lambda_{1}(z'_{11}; z'', z''')$$
(E.16)

of phases on the two paths takes the form

$$\Lambda_{-}(z'') = -S_{cl}(z''', T|z'_l) - S_{cl}(z'_l, T|z'') + S_{cl}(z'', T|z'_u) + S_{cl}(z'', T|z) + \hbar k(z'' - z'_l - z'_u + z). \quad (E.17)$$

Nowhere clearer than from the arguments of the classical actions do we see that the path is not closed. Indeed, reading from the right to the left we start from z and move via  $z'_u$  to z''. Then we go back via  $z'_1$  to z''' where  $z''' \neq z$ . We can only close the path by integrating over z''. However, for this purpose we have to use the explicit form of the classical actions.

Here two approaches offer themselves: (i) we recall the definitions (E.6), (E.10) and (E.11) of  $S_{\rm cl}$ ,  $z'_{\rm u}$  and  $z'_{\rm l}$ , substitute them into (E.17) and obtain in this way  $\Lambda_-$ ; (ii) we expand  $\Lambda_-$  into a Taylor series in z'' since  $S_{\rm cl}$ ,  $z'_{\rm u}$  and  $z'_{\rm l}$  depend on z'' at most quadratically. This approach leads us, together with the relations

$$\Lambda_{-}(z'')\Big|_{z''=0} = -\hbar kgT^2 = -\hbar \delta \varphi_g \tag{E.18}$$

and

$$\left. \frac{\partial \Lambda_{-}}{\partial z''} \right|_{z''=0} = \frac{m}{2T} (z''' - z) \tag{E.19}$$

as well as

$$\frac{\partial^2 \Lambda_-}{\partial (z'')^2} = 0 \tag{E.20}$$

to the explicit form

$$\Lambda_{-}(z'') = -\hbar \delta \varphi_g + (z''' - z) \frac{m}{2T} z''. \tag{E.21}$$

When we substitute this expression into (E.15) we find

$$M = e^{i\delta\phi} \frac{1}{2\pi} \int_{-\infty}^{\infty} d\zeta \ e^{i(z'''-z)\zeta} = e^{i\alpha} \delta(z'''-z), \tag{E.22}$$

that is M is diagonal, in complete agreement with the calculation of section 7. Here we have recalled the definition of  $\alpha$  and have introduced the integration variable  $\zeta \equiv mz''/(2\hbar T)$ .

### E.3. Connection to classical trajectories

It is interesting to compare and contrast the paths following from this stationary-phase-analysis of the quantum mechanical expression (E.1) for the matrix element with the classical trajectories obtained in section 3. Indeed, the considerations of the present appendix suggest the paths  $z \to z'_u \to z''$  on the upper arm of the interferometer and  $z''' \to z''_1 \to z''$  on the lower one, where  $z'_u$  and  $z'_1$  are given by (E.10) and (E.11), respectively.

We note that in table 1 the positions are expressed in terms of the initial position  $z_g(0)$  and velocity  $v_g(0)$  whereas in (E.10) and (E.11)  $z'_u$  and  $z'_1$  are given in terms of the initial and the final positions z or z''' and z'', respectively. We can connect the two approaches by eliminating  $v_g(0)$ . Indeed, we derive from the first row of the bottom part of table 1 the identities

$$z_{u}(T) = z_{g}(0) + v_{g}(0)T - \frac{1}{2}gT^{2} + \frac{\hbar k}{m}T$$
(E.23)

and

$$z_{\rm u}(2T) = z_g(0) + 2v_g(0)T - 2gT^2 + \frac{\hbar k}{m}T. \tag{E.24}$$

When we eliminate  $v_g(0)$  we arrive at

$$z_{\rm u}(T) = \frac{1}{2} \left[ z_{\rm u}(2T) + z_{\rm g}(0) \right] + \frac{\hbar k}{2m} T + \frac{1}{2} g T^2. \tag{E.25}$$

With the identifications  $z_g(0) \equiv z$  and  $z_u(2T) \equiv z''$  we find from (E.10) the relation  $z_u(T) = z'_u$ , that is the path selected by the method of stationary phase is indeed the classical one.

However, when we start from the second row of table 1 we find eliminating  $v_g(0)$  from the equations

$$z_{\rm I}(T) = z_g(0) + v_g(0)T - \frac{1}{2}gT^2$$
 (E.26)

and

$$z_1(2T) = z_g(0) + 2v_g(0)T - 2gT^2 + \frac{\hbar k}{m}T$$
(E.27)

the expression

$$z_{\rm I}(T) = \frac{1}{2} \left[ z_{\rm I}(2T) + z_{\rm g}(0) \right] - \frac{\hbar k}{2m} T + \frac{1}{2} g T^2$$
 (E.28)

which with the identifications  $z_g(0) \equiv z$  and  $z_u(2T) \equiv z''$  leads us to

$$z_l(T) \equiv \frac{1}{2}(z'' + z) - \frac{\hbar k}{2m}T + \frac{1}{2}gT^2.$$
 (E.29)

A comparison with the point of stationary phase  $z'_1$  given by (E.11) reveals that  $z_1(T) \neq z'_1$  unless z = z'''. As a result the lower path is, in general, not the classical one since they differ in their start points.

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