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Geometric potentials in quantum optics: A semi-classical interpretation

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Abstract. - We propose a semi-classical interpretation of the geometric scalar and vector potentials that arise due to Berry’s phase when an atom moves slowly in a light field. Starting from the full quantum Hamiltonian, we turn to a classical description of the atomic centre-of-mass motion while still treating the internal degrees of freedom as quantum variables. We show that the scalar potential can be identified as the kinetic energy of an atomic micro-motion caused by quantum fluctuations of the radiative force, and that the Lorentz-type force appears as a result of the motion-induced perturbation of the internal atomic state. For a specific configuration involving two counter-propagating Gaussian laser beams, we relate the geometric forces to the radiation pressure and dipole forces known from quantum optics. The simple physical pictures provided by the present analysis may help for the design and the implementation of novel geometric forces.

Cold atomic gases are considered as efficient simulators of quantum condensed matter systems (for a review, see e.g. [1]). The confinement potential and the atomic interactions can be tailored almost at will, allowing for example to mimic with atomic vapours situations encountered for electrons in solid state materials. A major step in the implementation of these simulators is the possibility to apply a gauge field to the cold atomic gas in order to model the vector potential appearing when charged particles are placed in a magnetic field. Up to now such gauge fields have been mostly obtained by rotating the gas [2]. In this case the transformation to the rotating frame indeed corresponds to giving the particles a fictitious charge, and applying an effective uniform magnetic field. Another method consists in using so-called geometric potentials which can considerably extend the range of gauge fields realisable in neutral gases. In particular, they offer the possibility to produce non homogeneous or time dependent effective orbital magnetism.

Geometric potentials [3–6] generally result from Berry’s phase [7] that appears when particles with an internal structure move slowly enough that their fast internal dynamics adiabatically adjusts to the centre-of-mass motion. In quantum optics such geometric potentials can be generated using laser beams to split the atomic internal energy levels. This was suggested in [8,9], and a first experimental investigation was presented in [10]. The concept of geometric potentials can be extended to simulate gauge fields that are more elaborate than the $U(1)$ symmetry of electromagnetism. Using appropriate laser configurations, one can in principle implement the general ideas outlined in [11] to generate non-Abelian gauge fields [12,13].

In spite of numerous investigations of possible geometric potentials in quantum optics, a simple physical interpretation of the forces appearing due to the gauge fields seems still to be lacking. Of course these forces ultimately arise from the exchange of momentum between light and atoms, but this generic process can lead to different physical mechanisms. Since identifying these mechanisms may help to design future configurations, we propose in this letter a semi-classical analysis of geometric potentials. Our approach is directly inspired by the formalism used to calculate the standard radiative forces acting on an atom placed in a laser beam. We first present the general semi-classical derivation of the two (scalar and vector) geometric potentials acting on an atom. We then discuss the various physical pictures that emerge for the concrete implementation that has been proposed in [14].

We start with a brief reminder of the standard formalism of geometric potentials, in which both internal and
external (centre-of-mass) atomic degrees of freedom are treated using quantum mechanics. The relevant internal dynamics is described in an $N$-dimensional Hilbert space. The atom can be submitted to static electric or magnetic fields as well as to time-dependent electromagnetic fields. The fields are supposed to be in a coherent state so that they can be described by classical functions. Assuming that the time-dependence of the atom-field interaction can be eliminated using the rotating-wave approximation, the eigenstates of the atom-field coupling form an orthogonal basis \{\ket{\psi_j(r)}, j = 1, \ldots, N\} of the internal Hilbert space of the atom at any point $r$. We denote $E_j(r)$ the corresponding energies. The Hamiltonian of the problem is thus

\begin{align}
\hat{H} &= \frac{\hat{p}^2}{2M} + \hat{V}(r) , \\
\hat{V}(r) &= \sum_{j=1}^{N} E_j(r) \hat{Q}_j(r) .
\end{align}

Here, $M$ is the atomic mass, $\hat{p} = -i\hbar \nabla$ the centre-of-mass momentum operator and $\hat{Q}_j(r) = |\psi_j(r)\rangle \langle \psi_j(r)|$ the projector onto the $j$-th internal eigenstate. Suppose now that the energy of one of the internal eigenstates, say $|\psi_1\rangle$, is well separated from the other ones. We choose the initial internal atomic state equal to $|\psi_1(r)\rangle$ at any point $r$ and suppose that the atom moves slowly enough for the adiabatic theorem to hold. The internal state then remains equal to $|\psi_1\rangle$ at any time, and the energy $E_1(r)$ plays the role of a potential energy for the centre-of-mass motion. In addition, the geometric phase accumulated by the atom gives rise to additional vector $A(r)$ and scalar $U(r)$ potentials so that the atom Hamiltonian in the adiabatic approximation [3–6] reads

\begin{align}
\hat{H}_{\text{adiab.}} &= \frac{(\hat{p} - A(r))^2}{2M} + E_1(r) + U(r) ,
\end{align}

with

\begin{align}
A(r) &= i\hbar \langle \psi_1(r)|\nabla \psi_1(r)\rangle , \\
U(r) &= \frac{\hbar^2}{2M} \sum_{j \neq 1} \langle \psi_1(r)|\nabla \psi_j(r)\rangle^2 ,
\end{align}

where we note by convention $|\nabla \psi(r)\rangle = \nabla (|\psi(r)\rangle)$.

The goal of this letter is to provide a simple physical interpretation of these potentials within the framework of a semi-classical analysis. Here, the term semi-classical refers to the fact that we describe the atomic internal degrees of freedom using quantum mechanics, but we treat classically the centre-of-mass motion. Within this approximation we want to recover the equation of motion

\begin{align}
M \frac{dv}{dt} &= -\nabla E_1(r) - \nabla U(r) + v \times B(r) ,
\end{align}

corresponding to the Hamiltonian \[\hat{H}\]. This equation of motion involves three forces. The first one is simply the gradient of the energy $E_1$ of the occupied level. The second one originates from the scalar potential $U(r)$, and the third one has the structure of a Lorentz force for a charge $q = 1$ in an effective magnetic field $B(r) = \nabla \times A(r)$.

The main tool for the semi-classical analysis is the force operator acting on the $N$-dimensional Hilbert space:

\begin{align}
\hat{F}(r) &= -\nabla \hat{V} = -\sum_j \left( \nabla (E_j) \hat{Q}_j + E_j \nabla (\hat{Q}_j) \right) .
\end{align}

Knowing the internal state $|\phi\rangle$ for an atom at point $r$ (a concept which is valid within the semi-classical approach), we will be able to calculate the average force $\langle \phi|\hat{F}(r)|\phi\rangle$ and the correlation functions of the force operator. This semi-classical approach has been very fruitful for the study of the radiative forces acting on an atom irradiated by laser beams [15], and its connection with a full quantum description of the atomic motion in laser light is well established [16].

**Origin of the scalar potential.** In this section we consider an atom with zero centre-of-mass velocity, so that the Lorentz force in (6) is also zero. The atom internal state is supposed to be $|\phi\rangle = |\psi_1\rangle$ and we immediately get from (8)

\begin{align}
\langle \hat{F}(r) \rangle &= -\nabla E_1 ,
\end{align}

where we used that the states $\{|\psi_j(r)\rangle\}$ form a normalised orthogonal basis at any point $r$. We thus recover the first term in eq. (8) but not the force originating from the scalar potential $U(r)$. This could be expected since the expression \[\hat{U}\] of the scalar potential involves the atomic mass $M$, which does not enter in the expression \[\hat{F}\] of the force operator $\hat{F}$. The scalar potential can still be recovered within the semi-classical approach, as we show now, provided one goes one step beyond the mere calculation of the average force.

The starting point of our reasoning consists in noting that the state $|\psi_1\rangle$ occupied by the atom is an eigenstate of the coupling Hamiltonian $\hat{V}$, but not an eigenstate of the force operator $\hat{F}$. Hence, $\langle \hat{F}^2 \rangle \neq \langle \hat{F} \rangle^2$ or, in physical terms, the force acting on the atom undergoes quantum fluctuations around its average value. As we will see, these fluctuations occur at the typical Bohr frequencies $\omega_{ij} = (E_j - E_i)/\hbar$ of the internal atomic motion. For the adiabatic approximation to hold, these frequencies have to be much larger than the characteristic frequencies of the external atomic motion. Consequently, the quantum fluctuations of the force cause a fast micro-motion of the atom, similar to the one arising for charged particles in a Paul trap [17]. The kinetic energy of the micro-motion then plays the role of a potential for the slow motion of the atomic centre-of-mass [18]. We demonstrate below that this kinetic energy coincides with the scalar potential $U(r)$.

The fluctuations of the force operator $\hat{F}$ are characterised by the symmetrised correlation function of the op-
erator $\delta \hat{F} = \hat{F} - \langle \hat{F} \rangle$, calculated in the Heisenberg picture:

$$C(t, t') = \frac{1}{2} \langle \delta \hat{F}(t) \cdot \delta \hat{F}(t') \rangle + \langle \delta \hat{F}(t') \cdot \delta \hat{F}(t) \rangle.$$  \hspace{1cm} (9)

Since the average is taken in an eigenstate of the Hamiltonian, $C(t, t')$ depends only on the time difference $\tau = t - t'$ and we obtain after some algebra

$$C(\tau) = \sum_{j \neq 1} C_j \cos (\omega_j \tau),$$

with

$$C_j = \hbar^2 \omega_j^2 |\langle \psi_1 | \nabla \psi_j \rangle|^2.$$ \hspace{1cm} (11)

In order to understand the consequences of these fluctuations, consider a classical particle submitted to a stochastic force $\mathbf{F}(t)$ such that $\mathbf{F}(t) = 0$ and $\mathbf{F}(t) \cdot \mathbf{F}(t') = C(t - t')$. The Fourier transform $\mathbf{f}(\omega)$ of $\mathbf{F}(t)$ is such that $\mathbf{f}(\omega) = 0$ and $\mathbf{f}(\omega) \cdot \mathbf{f}(\omega') = \delta(\omega - \omega') B(\omega)$, where

$$B(\omega) = \frac{1}{2} \sum_{j \neq 1} C_j \left( \delta(\omega + \omega_j) + \delta(\omega - \omega_j) \right)$$

is the Fourier transform of $C(\tau)$. The solution of the equation of motion $\mathbf{p} = \mathbf{F}$ is

$$\mathbf{p}(t) = \int \frac{\mathbf{f}(\omega)}{i\omega} e^{i\omega t} d\omega$$

and has a zero average. However, the average kinetic energy is strictly positive and equal to

$$\overline{\mathbf{p}^2} = \frac{1}{2M} \int \frac{B(\omega)}{2M \omega^2} d\omega.$$ \hspace{1cm} (14)

In the explicit calculation of [13], the contribution of the $\omega^{-2}$ denominator cancels out the transition frequencies $\omega_j$ that appear in the expression of $C_j$. Finally one exactly recovers the result [3] for the scalar potential. This validates the interpretation of this potential in terms of the kinetic energy of the atomic micro-motion. The above result sheds new light on the Hamiltonian [3] of the full quantum description. We can now interpret the term $M \ddot{\mathbf{v}}^2 / 2$, with $M \ddot{\mathbf{v}} = \mathbf{p} - \mathbf{A}$, as the kinetic energy of the slow centre-of-mass motion, whereas the kinetic energy of the fast micro-motion builds the scalar potential $U(\mathbf{r})$. It is also interesting to connect the present analysis of the scalar geometric potential with the intriguing problem of a two-level atom moving around the node of a standing wave. In the latter case, it is found that the average force acting on the atom is zero, as expected since the light intensity vanishes at the nodes. However, the atomic momentum diffusion coefficient, which is also related to the correlation function of the force operator, is non zero [15, 19].

**Origin of the Lorentz force.** – We now consider the case of a slowly moving atom and calculate the average of the force operator [1] at first order in velocity. More precisely, we assume an atom initially at rest in the internal state $|\phi\rangle = |\psi_1\rangle$, that is adiabatically set in motion to reach a velocity $\mathbf{v}$. Because of this motion the internal atomic state contains some admixture of the other eigenstates $|\psi_j\rangle$ and the average force is different from the zero-velocity result.

We write the internal state as $|\phi\rangle = \sum_j \alpha_j |\psi_j\rangle$ and solve the Schrödinger equation as a power series in velocity. The procedure detailed in the appendix gives the coefficients $\alpha_j$ at first order in $\mathbf{v}$:

$$\alpha_j(t) \simeq i \hbar \frac{\mathbf{v} \cdot (\psi_j | \nabla \psi_1 \rangle)}{E_j - E_1} e^{-i E_1 t / \hbar} \text{ (} j \neq 1 \text{).}$$ \hspace{1cm} (15)

The calculation of the average force at first order in $\mathbf{v}$ is also outlined in the appendix and leads to

$$\langle \delta \hat{F} \rangle = i \hbar \langle \nabla | \psi_1 \rangle (\mathbf{v} \cdot \nabla | \psi_1 \rangle) + \text{c.c.}$$ \hspace{1cm} (16)

One can readily check that this expression coincides with the Lorentz force $\mathbf{v} \times \mathbf{B}$ appearing in eq. [3].

This way of recovering the Lorentz force is very reminiscent of the general semi-classical calculation of the velocity-dependent radiative forces [15, 16]. There is one important difference, however. In the latter case one generally finds $\mathbf{F} \cdot \mathbf{v} \neq 0$, which is at the origin of laser cooling (for example via the Doppler or Sisyphus mechanisms). In the particular case considered here, no photon spontaneous emission process occurs, dissipation is absent, and we are left with a Lorentz force of geometric origin.

**Illustration for a particular atom-laser configuration.** – We now relate the geometric forces in quantum optics to the known radiative forces that generally act on an atom irradiated by one or several laser beams. We thus explain the mechanisms at the origin of the geometric potentials in terms of exchange of momentum between atoms and light. For this purpose, we turn to the specific configuration sketched in fig. [3] which has been proposed in [14]. A three-level atom with two degenerate ground states $|\alpha\rangle$ and an excited state $|\beta\rangle$ is irradiated by two counter-propagating laser beams. The beam propagating in the $+y$ (resp. $-y$) direction drives the transition $g_+ \leftrightarrow e$ (resp. $g_- \leftrightarrow e$). The two beams have the same waist $w$ and the same intensity. They are offset with respect to the $y$ axis by a distance $\pm b / 2$, where $b$ is typically of the order of $w$.

Using the rotating-wave approximation the atom-light coupling can be written as

$$\hat{V}(\mathbf{r}) = -\hbar \Delta |e\rangle \langle e| + \sum_{j=\pm} (\hbar \kappa_j(\mathbf{r}) |e\rangle \langle g_j| + \text{h.c.}).$$ \hspace{1cm} (17)

The Rabi frequencies $\kappa_\pm$ are given by

$$\kappa_\pm(\mathbf{r}) = \kappa e^{\pm iky} e^{-i(x^2+b^2)/w^2},$$ \hspace{1cm} (18)

where $k$ is the modulus of the wave vector of the laser beams. We assume that the Raman resonance condition is
satisfied between the two ground levels $g_\pm$, and we denote $\Delta$ the detuning of the laser frequency with respect to the $g_\pm \rightarrow e$ transition.

A well known characteristics of this configuration is that one of the three eigenstates of $\hat{V}(r)$ involves only the two ground states $|g_\pm\rangle$ and has zero overlap with the excited state $|e\rangle$ [20–22]. An atom prepared in this so-called non-coupled or dark state will not undergo any spontaneous emission process, which is a key feature for the practical use of geometric potentials. The non-coupled state is

$$ |\psi_1\rangle = \frac{\kappa_-}{\Omega} |g_+\rangle + \frac{\kappa_+}{\Omega} |g_-\rangle ,$$

where we set $\Omega = (|\kappa_-|^2 + |\kappa_+|^2)^{1/2}$. The corresponding energy at any point is $E_1(r) = 0$ so that the first term on the right hand side of (3) vanishes. The scalar potential and the effective magnetic field are [14]:

$$ U(x) = \frac{\hbar^2(k^2 + b^2/w^4)}{2M} G(x) ,$$

$$ B(x) = -\frac{2\hbar k b}{w^2} G(x) \mathbf{u}_x ,$$

where $G(x) = \cosh^{-2}(2xb/w^2)$.

We start our analysis with the scalar potential $U(r)$. When $x \rightarrow \pm \infty$, it tends to zero as expected from its interpretation as the energy of a micro-motion, which vanishes when the atom sits outside the laser beams. The value of $U$ at $r = 0$ can also be recovered easily. At this point the two components of the force operator are

$$ \hat{F}_x = -F_0 \left(|e\rangle\langle g_a| + |g_a\rangle\langle e|\right) ,$$

$$ \hat{F}_y = -iF_1 \left(|e\rangle\langle g_a| - |g_a\rangle\langle e|\right) ,$$

where $F_0 = \sqrt{2} \hbar k_b w^2$, $F_1 = \sqrt{2} \hbar k \kappa$ and where we have introduced the antisymmetric combination $|g_a\rangle = (|g_+\rangle - |g_-\rangle)/\sqrt{2}$. At $r = 0$, $|\psi_1\rangle = |g_a\rangle$ so that $\langle F_{x,y}\rangle = 0$, which directly follows from $E_1(r) = 0$. The correlation function of the force is readily calculated; choosing $\Delta = 0$ for simplicity, we find $C(\tau) = (F_0^2 + F_1^2) \cos(\sqrt{2}\kappa \tau)$. The kinetic energy of the micro-motion induced by this oscillating force is $(F_0^2 + F_1^2)/(4M\kappa^2)$ and indeed coincides with the general result (22) at $x = 0$. For realistic laser configurations the waist $w$ and the offset $b$ are large compared to $k^{-1}$ so that the dominating contribution is due to $F_1$, corresponding to a micro-motion directed along the propagation axis $y$ of the beams.

The two operators $\hat{F}_x$ and $\hat{F}_y$ given in (22, 23) are the so-called dipole force operator and radiation pressure force operator, respectively. The dipole force $\hat{F}_x$ originates from the intensity gradient of the laser beams along the $x$ axis.

In terms of photon momentum exchange, it can be understood as a redistribution of photons between the various plane waves that contribute to the formation of the intensity gradient (see e.g. [19]). The radiation pressure force $\hat{F}_y$ originates from the phase variation $e^{\pm ik_y y}$ of the laser beams along the $y$-axis. It leads to changes of atomic momentum by $\pm b k$ when the atom absorbs a photon from one of the laser beams. Interestingly, the cancellation of the average force acting on an atom at rest at $r = 0$ in the internal state $|g_a\rangle$ results from a destructive interference. For example, $\langle F_y \rangle = 0$ because the state $|g_a\rangle$ is a combination with equal weights of the two eigenvectors $|\chi_\pm\rangle = (|g_a\rangle \pm |e\rangle)/\sqrt{2}$ of the force operator $\hat{F}_y$. The dipole force felt by an atom in state $|\chi_\pm\rangle$ is $\mp F_0$, so that the average force vanishes for an atom prepared in $|g_a\rangle$.

We now turn to the case of a moving atom and to the interpretation of the Lorentz force. As the force is linear in velocity, we can study separately the cases of a motion parallel to the $x$ and to the $y$ axis. We first consider an atom moving along the $y$ axis with velocity $v_y$. Its internal state differs from the value $|g_a\rangle$ of an atom at rest, and its expression at first order in $v_y$, as deduced from (15), is

$$ |\phi\rangle = |g_a\rangle + \frac{kbv_y}{\sqrt{2}\kappa} |e\rangle ,$$

where we have again chosen $\Delta = 0$ for simplicity. This state can also be calculated directly by switching to the atom rest frame, which amounts to adding the small perturbation $\delta V = kv_y (Q_+ - Q_-)$ to the light-matter coupling, where $Q_\pm$ is the projector on the state $|g_\pm\rangle$. One can check that the state $|\phi\rangle$ is an eigenstate of the perturbed coupling $V + \delta V$ with the same eigenvalue 0. The average force acting on an atom in the state $|\phi\rangle$ is not zero anymore. The perfect balance between the two dipole forces $\pm F_0$ is now broken to the benefit of $-F_0 (\mp F_0)$ if $v_y > 0$. The explicit calculation of $\langle \phi|\hat{F}_y|\phi\rangle$ is immediate and yields exactly the Lorentz force value $-2\hbar kb v_y w^2$ obtained from eq. (22). In the case of a motion along the $y$ axis, the Lorentz force is therefore a direct consequence of the dipole potential. Remarkably, the Lorentz force is independent of the Rabi frequency $\kappa$ although the dipole force amplitude $F_0$ is proportional to $\kappa$. The reason is that the “rotation” angle of the state $|\phi\rangle$ with respect to the non-coupled state scales as $k^{-1}$ [see eq. (24)] and this scaling exactly compensates for the $k$ dependence of $F_0$.

We finally consider an atomic motion along the $x$ axis, with a Lorentz force along the $y$-axis, originating thus from the radiation pressure force operator $\hat{F}_y$. This case could be analysed along the lines of eqs. (22, 23), but it is actually more instructive to look at the cumulative effect of the
Lorentz force, i.e. the change of momentum along $y$, when the atom crosses the two laser beams. Suppose that the atom is initially located at time $t_1$ at a position $x_1 < 0$ with $|x_1| \gg w$. At this location $\kappa/+\kappa=\exp(2x_1b/w^2) \ll 1$, so that eq. (23) leads to $|\psi_1| \simeq |g_+\rangle$. At a later time $t_2$ the atom has reached the point $x_2 = -x_1$, where $|\psi_1| \simeq |g_-.\rangle$. The momentum change caused by the Lorentz force is aligned with the $y$ axis and its value is

$$\Delta p_y = -\int_{t_1}^{t_2} B_z v_x \, dt = -\int_{x_1}^{x_2} B_z(x) \, dx$$

$$= \hbar k \left[ \tanh(2x_2b/w^2) - \tanh(2x_1b/w^2) \right] \quad (25)$$

With the above assumption that $|x_1| = |x_2| \gg w$ and $b \sim w$, we obtain

$$\Delta p_y \simeq 2\hbar k \quad (26)$$

This expression has a clear physical interpretation in terms of photon absorption and stimulated emission. When the atom moves from $x_1$ to $x_2$, its internal state rotates adiabatically from $|g_+\rangle$ to $|g_-\rangle$. This happens by the absorption of a photon from the wave propagating in the $+y$ direction, driving the $g_+ \to e$ transition, and the stimulated emission of a photon in the wave propagating in the $-y$ direction, driving the $e \to g_-$ transition. The origin of the Lorentz force in this case is therefore closely related to the so-called STIRAP process (Stimulated Raman Adiabatic Passage) [23].

**Discussion and conclusion.** We have given here a semi-classical interpretation of the geometric forces that act on a slowly moving particle with multiple, spatially varying, internal energy levels. Such a situation is encountered in quantum optics when an atom moves in the light field created by several quasi-resonant laser beams. The main assumption is that the atom follows adiabatically one of its internal energy levels which is supposed to be well separated from all the other ones. Under these conditions the atomic centre-of-mass motion involves a scalar and a vector potential. The scalar potential originates from the kinetic energy of the micro-motion of the atom, under the action of the quantum fluctuations of the radiative force operator. The Lorentz-type force associated with the vector potential results from the perturbation of the atomic internal state due to the slow atomic motion. This changes the expectation value of the force with respect to an atom at rest, but does not induce any dissipation. The way we obtain our results is very reminiscent of the general derivation of the radiative forces created by quasi-resonant laser beams. Taking as an example the configuration proposed in [14], we have related the intervening geometric forces with either the radiation pressure force or the dipole force.

Our approach can be viewed as a quantum version (for the internal degrees of freedom) of the fully classical results of [24], where the authors analysed the motion of a particle with a permanent magnetic moment placed in a strong, non homogenous magnetic field. There, a rapid oscillation of the magnetic moment superimposed onto a slow secular motion was found. This rapid oscillation gives rise to a scalar potential similar to the one of interest here. When the particle with its magnetic moment initially aligned with the magnetic field was set in motion, it was found that the magnetic moment acquires a non-zero component in a direction perpendicular to the magnetic field. The Lorentz-type force that emerged in this situation is also very similar to the present one.

To conclude, geometric potentials may constitute in the future a key ingredient for the realisation of a general ‘quantum gas toolbox’ that allows one to address various open problems of many-body physics. We hope that the simple physical pictures provided by the present analysis may help for the design and the implementation of novel geometric forces in this context.

**Appendix: Derivation of the Lorentz force.** In this appendix we detail the calculation of the perturbed state $|\phi\rangle$ of a slowly moving atom and the resulting force $\langle \hat{F} \rangle$. At time 0 the atom is at rest in the internal state $|\phi\rangle = |\psi_1\rangle$. We suppose that it is uniformly accelerated during a time $T$ to a velocity $v$: $v(t) = v\, t/T$ for $0 \leq t \leq T$. Our aim is to calculate $|\phi\rangle$ and $\langle \hat{F} \rangle$ at time $T$.

The general expression of the internal atomic state is $|\phi(t)\rangle = \sum_j \alpha_j(t) |\psi_j(r(t))\rangle$, which, leading to the average of the force operator $\langle \hat{F} \rangle$:

$$\langle \hat{F} \rangle = -\sum_j \nabla E_j \, |\alpha_j|^2 \quad + \sum_{j,k} (E_k - E_j) \, \alpha_j^* \alpha_k \, \langle \psi_k | \nabla \psi_j \rangle \quad (27)$$

To calculate the force at first order in $v$, we need all coefficients $\alpha_j$ also at first order. Using the Schrödinger equation $i\hbar |\dot{\phi}\rangle = \hat{V}(r(t)) |\phi\rangle$ and $|\phi\rangle = \sum_j \alpha_j |\psi_j\rangle$, we get the corresponding equations of motion:

$$\dot{\alpha}_j = -iE_j \alpha_j / \hbar + \sum_k \alpha_k \, v \cdot \langle \psi_j | \nabla \psi_k \rangle \quad (28)$$

At order zero all $\alpha_j$’s are zero except $\alpha_1(t) = \exp(-iE_1 t/\hbar)$. At order one we obtain for $j \neq 1$

$$\alpha_j(T) = -v \cdot \langle \psi_j | \nabla \psi_1 \rangle \, e^{-iE_1 T/\hbar} \int_0^T e^{i(E_j - E_1)t/\hbar} \, t \, dt \quad (29)$$

where $|\psi_j\rangle$, $|\psi_1\rangle$, $E_j$ and $E_1$ are taken at order zero in $v$, hence at the location $r$ of the atom at time $T$. Assuming that the atom is adiabatically set into motion, i.e. $T(E_j - E_1)/\hbar \gg 1$, we get

$$\alpha_j(T) \simeq i\hbar \, v \cdot \langle \psi_j | \nabla \psi_1 \rangle \, e^{-iE_1 T/\hbar} \quad (30)$$

At order one in $v$ the equation of motion for $\alpha_1$ is

$$\dot{\alpha}_1 = -i(E_1 - v \cdot A) \alpha_1 / \hbar \quad (31)$$

whose solution is a number of modulus 1. The two results ([22]) and ([23]) entail that the first part of $\langle \hat{F} \rangle$ in ([27]) has
no first order component in $v$ since the contributions of the $\alpha_j$'s for $j \neq 1$ are at least of order 2, and the contribution of $\alpha_1$ is independent of $v$. In the second part of (23), the only relevant terms are those where one of the two indices $k$ or $j$ equals 1. Applying the closure relation and keeping the terms linear in velocity, we finally reach the result \[ R \] for the average force. We note that our procedure is similar to the original derivation of the geometric phase \[7\], which emerges from the term $v \cdot A$ in (31).

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