Free Space Quantum Walk of Neutral Atoms in a Propagating Light

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We demonstrate that a coherent propagating light causes quantum walk of a neutral atom with tunable step length in free space without optical lattice. This effect further induces optical Stern-Gerlach effect in propagating light. The momentum exchange induced optical force is repulsive for the ground state atom and attractive for the excited state atom. The motion of atom wave packets are described by Schrödinger equation with analytical solutions and an experimental design for verification of this effect is given. These results may important for the development of atomtronics, quantum information processing and topological effects in atomic gas.

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How atoms move in electromagnetic fields is a fundamental problem. Interaction between atom and light is inevitably accompanied by momentum exchange and corresponding impulsive forces [1, 2], which can be used in atom cooling [3, 5] and atom trapping [6, 8]. These techniques play important role in the realization of Bose-Einstein condensation [9, 11] and optical lattice [12, 14]. In long coherent time atom-light interactions, such as Raman transitions or clock transitions, artificial gauge field and spin-orbit coupling can be generated [13, 16].

Couplings between momentum and internal states of quantum particles play important role in the generation of quantum walks, which have wide applications in the implementation of quantum computations [17, 21] and topological phase transitions [22, 26]. Quantum walks describe the motion of particles whose localizations depend on quantum coins [27]. Photons [28, 30], ions [31, 33] and neutral atoms [34, 41] can be used to observe quantum walks. Until now, as we know, all these neutral atom based quantum walks require optical lattice.

In this paper, we first show that a propagating coherent light could induces quantum walk of a neutral atom in free space without the requirement of optical lattice. Due to momentum conservation during the coherent process of light emission and absorption, effective optical force is repulsive for the ground state atom and attractive for the excited state atom as illustrated in Fig. 1 (a)-(c). It is similar to electric force acting on positive and negative charge. Different from the continuous motion of charged particle in electrostatic field, displacement of the neutral atom in propagating light is quantized with a definite step length as schematically shown in Fig. 1 (d)-(f).

Advantage of the free space quantum walk is that quantum walk based systems would not rely on periodic potentials such as optical lattice. Furthermore, similarities between the atomic motion in propagating light and charged particles in electromagnetic field can make the free space quantum walk effect have potential applications in atomtronics. Atomtronics is an emerging technique in cold atom systems [19, 34], in which atoms are believed to controllable and useful analogous to electrons in electronics.

Hamiltonian of a single two-level atom coupled to a linearly polarized monochromatic running wave light \( \vec{E}(x, t) = \epsilon z E_0 \cos(\omega t - kx + \phi_0) \) could be written as [1, 3, 4]

\[
\mathbf{H} = \mathbf{H}_e + \frac{p^2}{2M} - \epsilon z E_0 \cos(\omega t - kx + \phi_0),
\]

where \( \mathbf{H}_e \) represents electronic energy of the atom, \( \frac{p^2}{2M} \) is kinetic energy of the center of mass of the atom with the atom mass \( M \), and the third term denotes dipole interaction between the atom and the propagating light field \( \vec{E}(x, t) \).

For a non-interacting atom, eigenstate and eigenenergy of internal electronic motion is defined as \(|n\rangle\) and

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FIG. 1: (Color on line) (a)-(c) The relation of momentum conservation during the atom-light interaction within the half periodicity \( T/2 \). (d)-(f) Quantum walk of an atom with the displacement step \( \Lambda \) and periodicity \( T \).
Then we have $H_1|n\rangle = \varepsilon_n|n\rangle$, $n = 0, 1$. In the same way, momentum operator $p$ satisfies $p|p\rangle = p|p\rangle$ for the momentum eigenstate $|p\rangle$. Using the momentum displacement operator $e^{\pm i k x}|p\rangle = |p \pm \hbar k\rangle$ in the Hilbert space of non-interacting eigenstates $\{|n, p\rangle\}$ \[\mathcal{H}\]. Hamiltonian (1) with the rotating wave approximation should be written as

$$H = \sum_{n=0,1} \varepsilon_n |n\rangle \langle n| + \int dp \frac{p^2}{2M} |p\rangle \langle p|$$

$$-\frac{\hbar}{2} \int dp (\Omega(t)|0, p + \hbar k\rangle \langle 0, p| + \Omega^*(t)|0, p - \hbar k\rangle \langle 1, p|),$$

(2)

where $\Omega(t) = \Omega e^{-i(\omega t + \phi)}$ and the Rabi frequency is $\Omega = |\mu|E_0/h$ with dipole moment of the atom $\mu = (0|e|x|1) = |\mu|e^{i\phi_0}$ \[\mathcal{H}\]. The phase $\phi = \phi_0 + \phi_1$ includes initial phases of the atom and the light. The initial phase would be taken to be $\phi = 0$ for convenience of discussion.

Motion of the single atom should be described by the Schrödinger equation $i\hbar \frac{\partial}{\partial t} |\Psi(t)\rangle = H|\Psi(t)\rangle$. The unitary operator $e^{iH_0 t/\hbar}$ \[\mathcal{H}_0 = \varepsilon_0|0\rangle \langle 0| + (\varepsilon_0 + \hbar \omega)|1\rangle \langle 1|\] helps us to transform the Schrödinger equation into the form of interaction picture

$$i\hbar \frac{\partial}{\partial t} |\varphi(t)\rangle = V|\varphi(t)\rangle,$$

(3)

where $|\varphi(t)\rangle = e^{iH_0 t/\hbar} |\Psi(t)\rangle$ and $V = e^{iH_0 t/\hbar} He^{-iH_0 t/\hbar}$ becomes time-independent Hamiltonian. The wave function $|\varphi(t)\rangle$ can be expanded with probability distribution functions as $|\varphi(t)\rangle = \int dp \sum_n \varphi_n(p, t)|n, p\rangle$, where $\varphi_n(p, t)$ is in fact $\varphi_n(p, t) = C_n \varphi_p(t, p)$. Here, $C_0$ and $C_1$ are probability amplitudes of the atom electronic states $|0\rangle$ and $|1\rangle$, respectively. For a definite momentum $p$, Eq. (3) can be written in a $2 \times 2$ sub space as $i\hbar \frac{\partial}{\partial t} |\varphi_p(t)\rangle = V(p)|\varphi_p(t)\rangle$, where $|\varphi_p(t)\rangle = \varphi_0(p, t) + \varphi_1(p + \hbar k, t)$. Then we have $C_0 = 1$ and $C_1 = 0$. Other parameters are $p_c = 0$, $\Pi/\hbar k = 2$. The phase with dipole moment of the atom $\varphi_{1p}(t)|0, p\rangle + \varphi_{1p+hk}(t)|1, p + \hbar k\rangle$ and the Hamiltonian $V(p)$ becomes

$$V(p) = \begin{pmatrix} \frac{\hbar^2}{2M} & -\frac{\hbar^2}{2} \hbar \Delta + \frac{(p + \hbar k)^2}{4M} \\ -\frac{\hbar^2}{2} \hbar \Delta + \frac{(p + \hbar k)^2}{4M} & \frac{\hbar^2}{2M} \end{pmatrix}.$$  

(4)

Diagonalization of the Hamiltonian $V(p)$ can be easily carried out with the transformation matrix $U$,

$$U = \begin{pmatrix} \sqrt{A+1} & \sqrt{A+1} \\ \sqrt{B+1} & \sqrt{B+1} \end{pmatrix},$$

(5)

where $A = \frac{b-a+\sqrt{(b-a)^2+4J^2}}{2J}$, $B = \frac{b-a-\sqrt{(b-a)^2+4J^2}}{2J}$, $a = \frac{\hbar^2}{2M}$, $b = \Delta + \frac{(p + \hbar k)^2}{4M}$ and $J = \frac{\Omega^2}{2}$. The diagonalized Hamiltonian $h\hat{W} = U V(p) U^\dagger$ satisfies $W\hat{\Phi}_j(p, t) = \hat{W}_j \hat{\Phi}_j(p, t)$, with the eigenvalues $h\hat{W}_0 = \frac{1}{2} \sqrt{(a + b + \sqrt{(a-b)^2+4J^2})}$, $h\hat{W}_1 = \frac{1}{2} \sqrt{(a + b - \sqrt{(a-b)^2+4J^2})}$, and corresponding eigenvectors are $\hat{\Phi}_j(p, t) = \hat{\Phi}_j(p, t)|\Phi_j\rangle$, $j = 0, 1$. $\Phi_j(p, t)$ can be obtained directly from the diagonalized Schrödinger equation $i\hbar \frac{\partial}{\partial t} \hat{\Phi}_j(p, t) = \hat{W}_j \hat{\Phi}_j(p, t)$ in the form $\hat{\Phi}_j(p, t) = \hat{\Phi}_j(0, p)e^{-i\hat{W}_j t}$. Since the eigenvector $|\Phi_j(p, t)\rangle = \hat{\Phi}_j(p, t)|\Phi_j\rangle$ satisfies $\hat{\Phi}_j(p, t) = U|\varphi_p(t, p)\rangle$, the initial state can be determined by $|\varphi_p(0, 0)\rangle = U|\varphi(0, 0)\rangle$. Then, we obtain the original wave function $|\varphi_p(t, p)\rangle = U|\Phi_j(p, t)\rangle$ for a given initial condition $|\varphi(0, 0)\rangle$. In the initial wave function $|\varphi(0, 0)\rangle = \varphi_{0p}(0, p) + \varphi_{1p+hk}(0, 1, p + \hbar k)$, we have $\varphi_{0p}(0) = C_0 \varphi_p(0, 0)$ and the probability distribution is given by Gaussian function $\varphi_p(0, 0) = \frac{1}{\pi \hbar^2} e^{-\left(p - p_c\right)^2/2\hbar^2}$, where $p_c$ is the center momentum and $\Pi$ is the characteristic momentum. In the following numerical treatment, we take Strontium ($^{87}\text{Sr}$) atom as a sample. $^{87}\text{Sr}$ atom is characterized by its mass $M = 86.9088775u$ ($u =$
of atom momentum is very small.

\[ \Delta = 0 \] and the optical force acting on the atom \( F(t) \) can be calculated through the formula \( \langle p(t) \rangle = \langle \varphi(t) | p | \varphi(t) \rangle \).

From the function of momentum \( \langle p(t) \rangle \) we can obtain displacement of the atom \( \langle x(t) \rangle = \langle x(0) \rangle + \int_0^t F(t') dt' \) and the optical force acting on the atom \( F(t) = \frac{\hbar}{\pi} \langle p(t) \rangle \).

For convenience of discussion, we write the three quantities in their simple forms. In the strong coupling regime \( \Omega \gg \delta \), they can be simplified as

\[ \langle p(t) \rangle = p_c + (C_0^2 - C_1^2) \hbar \sin^2 \left( \frac{\Omega t}{2} \right), \]

with the momentum amplitude \( \hbar k \),

\[ \langle x(t) \rangle = \langle x(0) \rangle + \frac{2p_c}{\hbar k} \Lambda \Omega t + (C_0^2 - C_1^2) \Lambda (\Omega - \sin(\Omega t)), \]

with the step length \( \Lambda = \frac{\hbar k}{2M\Omega} \), and

\[ \langle F(t) \rangle = (C_0^2 - C_1^2) F_0 \sin(\Omega t), \]

with the force amplitude \( F_0 = \frac{1}{2} h k \Omega \). In addition, probability distribution of the atom wave packet in momentum space \( |\varphi(p, t)\rangle^2 \) satisfies the relations about the normalization condition \( \langle \varphi(t) | \varphi(t) \rangle = 1, \langle \varphi(t) | \varphi(t) \rangle = \int dp \sum_n |\varphi_n(p, t)\rangle^2 \) and \( |\varphi(p, t)\rangle^2 = \sum_n |\varphi_n(p, t)\rangle^2 \). Wave function in position space can be obtained using the Fourier transformation \( |\psi(x, t)\rangle = (x | \varphi(t) \rangle) \).

For the wave function here \( |\varphi(t)\rangle = \int dp (\varphi_0(p, t) |0\rangle + \varphi_1(p, t) |1\rangle) \), we have \( |\psi(x, t)\rangle = \psi_0(x, t) |0\rangle + \psi_1(x, t) |1\rangle \), where the amplitudes can be calculated through \( \psi_0(x, t) = \int dp \varphi_0(p, t) \langle x | p \rangle \) and \( \psi_1(x, t) = \int dp \varphi_1(p, t) \langle x | p \rangle \).

In Fig. 3(a)-(d), a static atom \( p_c = 0 \) with the characteristic momentum \( \Pi = 0.5 \hbar k \) set to be in its ground state \( |0\rangle \) initially. The static atom get a momentum \( \hbar k \) at time \( \frac{\pi}{\Omega} \) and stop at time \( \frac{3\pi}{\Omega} \) by losing the momentum \( \hbar k \).

As shown in Fig. 4 the atom moves and stop with the periodicity \( T \) and step length \( \Lambda \). The step length \( \Lambda \) determined by atom mass, light frequency and their coupling rate. When the atom is in the excited state \( |1\rangle \) initially, the same behavior should be observed but in the opposite direction as illustrated in Fig. 3(e)-(h). Clearly, the direction of atom motion depends on the initial state.
It also can be explained from Eq. 5, the optical forces \( \langle F(t) \rangle \) which starts from positive value for a ground state atom and negative for an excited state atom analogous to the electric force on charged particle.

Atom in the superposition state \( |\varphi(0)\rangle = \int dp \varphi(p, 0)(C_0|0\rangle + C_1|1\rangle)|p\rangle \) leads to atom walk in superposition of different directions. In Fig. 5 the atom is assumed to be initially set in the superposition state \( \int dp \varphi(p, 0)(\frac{1}{\sqrt{\pi}}|0\rangle + \frac{1}{\sqrt{\pi}}|1\rangle)|p\rangle \). After half periodicity \( T/2 \), wave packet in the amplitude \( \frac{1}{\sqrt{\pi}}|0\rangle \) transits into the state \( \frac{1}{\sqrt{\pi}}|1\rangle \) with averaged momentum \( \frac{\hbar}{2\pi} \), at the same time, wave packet in the amplitude \( \frac{1}{\sqrt{\pi}}|1\rangle \) transits into the state \( \frac{3}{\sqrt{\pi}}|0\rangle \) with averaged momentum \( \frac{9\hbar}{25\pi} \), and the total atom gains momentum \( \frac{7\hbar}{25\pi} \) as plotted in Fig. 5 (b). Due to momentum conservation, the atom emits a photon with averaged momentum \( \frac{\hbar}{2\pi} \) which is in accord with the interaction process show in Fig. 1 (c). The momentum space wave packet distribution in Fig. 5 (a) has been plotted in Fig. 6 along the time change. Wave function evolution in position space is shown in Fig. 7 in which the atom is in a superposition states of counter propagating wave packets. Wave packet in the ground state \( |0\rangle \) is propagating in \( x \) direction with step length \( \frac{16\Lambda}{9\pi} \) and wave packet in the excited state \( |1\rangle \) is propagating in \(-x\) direction with step length \( \frac{5\Lambda}{9\pi} \), respectively (also see Fig. 1 (f)). The quantum walk in superposition states, should be applied to observe optical Stern-Gerlach effect in propagating light, which was observed early in standing wave light [42].

Finally, we consider more general case in which an atom has non-zero initial velocity, \( p_c \neq 0 \). When an atom is initially moving with the center momentum \( p_c = -0.5\hbar k \) and electronic state \( |0\rangle \), it would oscillate around the original position \( \langle x(0) \rangle \) as shown in Fig. 5 (a) and (b). From the wave packet distribution, one can know that center momentum of the atom is changing between \(-\hbar k/2\) and \( \hbar k/2 \) with the periodicity \( T \). The oscillation also occur for an atom in initial state \( p_c = 0.5\hbar k \) and \( |1\rangle \) as shown in Fig. 5 (c) and (d). For a faster moving atom with a momentum \( p_c = 5\hbar k \) along the light propagation, displacement of the atom would be \( 5\pi \Lambda \) during the time \( t = 5T \). In contrast, a counter propagating atom with initial center momentum \( p_c = -5\hbar k \), its displacement within the time is \( 45\Lambda \). The former is accelerated and the latter is decelerated as shown in Fig. 5 (c) and (f). We may conclude a formula describing displacement \( \Delta x_n(N) \) of an wave packet in state \( n \rangle \) within an integral periodicity,

\[
\Delta x_n(N) = \left( \frac{2p_c}{\hbar k} + (-1)^n C_n^2 \right) N\Lambda,
\]

where \( N \) is the number of periodicity. For the fast atom as plotted in Fig. 5 (c) and (g), walking steps of the atom cannot observed obviously.

For observation of the quantum walk, we designed an experimental set up in Fig. 9. Laser width is set to be...
L and entered atoms move only in y direction with velocity $v_y$. If the width $L$ and speed $v_y$ are set to satisfy $L/v_y = N\frac{\Delta x}{\Delta y}$ ($N$ is integer), one knows from Eq. (9) that momentum of the atom in x direction should become zero when the atom leaves the laser field. In this case, Eq. (9) reveals that the positions of deflected atoms expected to be $x_0 = N\Delta x$ in experiment (a), $x_1 = -N\Delta x$ in experiment (b), $x_0 = -N\Lambda/2$ and $x_1 = N\Lambda/2$ in experiment (c). With the parameters of $^{87}$Sr atom and Rabi frequency $\Omega = 100$ KHz, the step length is approximately $\Lambda \approx 33$ nm. Challenge of this experiment may be how to obtain the atom beam with pure velocity and atom detection with high precision.

In summary, we proposed a theoretical model of fully coherent coupling between an ultra-slow atom and a propagating light, which exploit quantum walk with tunable step length in free space. Here, we give several outlooks. 1. The quantum walk of single atoms may have applications for the realization of nanometer to micrometer scaled atom beam splitter. 2. Measurement of electronic levels and dipole moments of atoms through the propagating light induced quantum walk and Stern-Gerlach deflection is possible. 3. The free space quantum walk of atoms in two or three dimensional free space can be predicted here. 4. The repulsive and attractive force generated from the coherent coupling between running wave light and neutral atoms may play important role for the development of artificial gauge field in cold atoms, atomtronics and related applications.

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[1] R. J. Cook, Phys. Rev. Lett. 41 (1978) 1788.
[2] J. Dalibard and C. Cohen-Tannoudji, J. Opt. Soc. Am. B 2 (1985) 1707.
[3] H. Metcalf and P. van der Straten, Phys. Rep. 244 (1994) 203.
[4] C. S. Adams and E. Riis, Progress in Quantum Electronics 21 (1997) 1.
[5] W. D. Phillips, Rev. Mod. Phys. 70 (1998) 721.
[6] E. L. Raab, M. Prentiss, A. Cable, et al., Phys. Rev. Lett. 59 (1987) 2631.
[7] O. Zobay and B. M. Garraway, Phys. Rev. Lett. 86 (2001) 1195.
[8] V. I. Balykin, K. Hakuta, F. Le Kien, et al., Phys. Rev. A 70 (2004) 011401.
[9] M. H. Anderson, J. R. Ensher, M. R. Matthews, et al., Science 269 (1995) 198.
[10] C. C. Bradley, C. A. Sackett, J. J. Tollett, et al., Phys. Rev. Lett. 75 (1995) 1687.
[11] K. B. Davis, M.-O. Mewes, M. R. Andrews, et al., Phys. Rev. Lett. 75 (1995) 3969.
[12] D. Jaksch, C. Bruder, J. I. Cirac, et al., Phys. Rev. Lett. 81 (1998) 3108.
[13] M. Köhl, H. Moritz, T. Stöferle, et al., Phys. Rev. Lett. 94 (2005) 080403.
[14] M. Greiner and S. Fölling, Nature 453 (2008) 736.
[15] J. Dalibard, F. Gerbier, G. Juzeliūnas, Rev. Mod. Phys. 83 (2011) 1523.
[16] L. F. Livi, G. Cappellini, M. Diem, et al., Phys. Rev. Lett. 117 (2016) 220401.
[17] N. Shen, J. Kempe, and K. B. Whaley, Phys. Rev. A 67 (2003) 052307.
[18] A. M. Childs, D. Gosset, and Z. Webb, Science 339 (2013) 791.
[19] P. Chawla, R. Mangal, and C. M. Chandrashekar, Quantum. Inf. Process. 19 (2020) 158.
[20] G. A. Bezerra, P. H. G. Lugão, and R. Portugal, Phys. Rev. A 103 (2021) 062202.
[21] S. Singh, P. Chawla, A. Sarkar, et al., Sci. Rep. 11 (2021) 11551.
[22] M. S. Rudner and L. S. Levitov, Phys. Rev. Lett. 102 (2009) 065703.
[23] T. Kitagawa, M. Broome, A. Fedrizzi, et al., Nat. Commun. 3 (2012) 882.
[24] J. K. Asbóth, Phys. Rev. B 86 (2012) 195414.
[25] F. Cardano, A. D’Errico, A. Dauphin, et al., Nat. Commun. 8 (2017) 15516.
[26] V. Mittal, A. Raj, S. Dey, et al., Sci. Rep. 11 (2021) 10262.
[27] Y. Aharonov, L. Davidovich, and N. Zagury, et al., Phys. Rev. A 48 (1993) 1687.
[28] D. Bouwmeester, I. Marzoli, G. P. Karman, et al., Phys. Rev. A 61 (1999) 013410.
[29] M. A. Broome, A. Fedrizzi, B. P. Lanyon, et al., Phys. Rev. Lett. 104 (2010) 153602.
[30] A. Crespi, R. Osellame, R. Ramponi, et al., Nature Photon. 7 (2013) 322.
[31] B. C. Travaglione and G. J. Milburn, Phys. Rev. A 65 (2002) 032310.
[32] H. Schmitz, R. Matjeschk, C. Schneider, et al., Phys. Rev. Lett. 103 (2009) 090504.
[33] F. Zähringer, G. Kirchmair, R. Gerritsma, et al., Phys. Rev. Lett. 104 (2010) 100503.
[34] W. Dirr, R. Raussendorf, V. M. Kendon, et al., Phys. Rev. A 66 (2002) 052319.
[35] M. Karski L. Förster, J.-M. Choi, et al., Science 325 (2009) 174.
[36] C. Weitenberg, M. Endres, J. F. Sherson, et al., Nature 471 (2011) 319.
[37] P. M. Preiss, R. Ma, M. E. Tai, et al., Science 347 (2015) 1229.
[38] U. Schneider, L. Hackermuller, J. Ronzheimer, et al., Nature Photon. 8 (2012) 213.
[39] M. Genske, W. Alt, A. Steffen, et al., Phys. Rev. Lett. 110 (2013) 190601.
[40] T. Fukuhara, P. Schauß, M. Endres, et al., Nature 502 (2013) 76.
[41] S. Rylands and N. Andrei, Phys. Rev. B 100 (2019) 064308.
[42] T. Sleator, T. Pfau, V. Balykin, et al., Phys. Rev. Lett. 68 (1992) 1996.
[43] R. A. Pepino, J. Cooper, D. Z. Anderson, et al., Phys. Rev. Lett. 103 (2009) 140405.
[44] S. Eckel, J. Lee, F. Jendrzejewski, et al., Nature 506 (2014) 200.
[45] K. W. Wilsmann, L. H. Ymai, A. P. Tonel, et al., Commun. Phys. 1 (2018) 91.
[46] W. Lai, Y.-Q. Ma, L. Zhuang, et al., Phys. Rev. Lett. 122 (2019) 223202.
[47] Y. Winsten and D. Cohen, Sci. Rep. 11 (2021) 3136.
[48] P. Meystre and M. Sargent III, Elements of Quantum Optics, Springer-Verlag, Berlin/Heidelberg/New York, 2007
[49] M. O. Scully and M. S. Zubairy, Quantum Optics, Cambridge University Press, Cambridge, 1997
[50] G. K. Campbell, A. D. Ludlow, S. Blatt, et al., Metrologia 45 (2008) 539.