Optical Purification of Materials via Electromagnetically Induced Walking

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Natural materials are always mixed with foreign matters which affect their physical or chemical properties. Here, we give an optical method for the precise purification of gaseous state materials. Principle of this method is originated from spin-orbit coupling in electromagnetically induced walking where fingerprints of atoms such as masses and optical transition wavelengths determine walking speed of the atoms. This method could be used for some hardly separable atoms and isotopes depending on the condition of atom coherent time. The present work opens a platform for applications of cold atom technology in the purification of atoms and molecules.

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Material purification is the physical separation of a chemical substance of interest from foreign or contaminating substances. It plays important role in many fields such as medicine, chemistry, manufacturing and micro-fabrication. Especially the material challenges are limiting urgent progress in frontier technology, for example, quantum computing hardware platforms [1], single photon sources [2], high-temperature superconductivity [3, 4], semiconductor quantum dots [5] and so on. There are many well developed methods of material purification, such as filtration, centrifugation, evaporation, extraction, crystallization, adsorption, smelting, distillation, downstream processing, water purification, fractionation and electrolysis.

In this letter, we propose an optical method of purification based on the electromagnetically induced walking (EIW) [6]. In EIW, an atom would coherently walk along the direction of propagating light and the velocity of the atom is related to the atom mass and its optical transition wavelength. This property has potential application in the separation and purification of materials, especially for the achievement of high purely nano materials. Taking advantages of the well developed cold atom beam experiments [6–8], the present quantum mechanical method should be feasible in practice.

Theoretical model of setup for the optical purification is conceptually shown in Fig. 1 (a). Here, we just consider diluted cold atoms where atom-atom interactions could be neglected [10, 11]. Hamiltonian of any individual atom

![Image](a) Schematic illustration of separation and purification. (b) Electromagnetically induced walking in the synthetic dimensions of atom.

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The atom-light detuning $\Delta = |\epsilon|$, solved through the Schrödinger equation

$$i\hbar \frac{\partial \Psi(t)}{\partial t} = H\Psi(t),$$

where the wave function $|\Psi(t)\rangle$ of the atom could be solved through the Schrödinger equation $i\hbar \frac{\partial}{\partial t} |\psi(t)\rangle = V|\psi(t)\rangle$, where the wave function can be expanded with probability distribution functions as $|\psi(t)\rangle = \int dp \sum_n \varphi_n(p,t)|n,p\rangle$. $V$ is a time independent Hamiltonian and it can be diagonalized in a subspace of definite momentum $p$. The eigenfrequencies are $W_{0,1} = \frac{1}{\hbar}(\omega_p + \omega_{p+hk} + \Delta \mp \Sigma)$, in which the transition frequency in interaction picture is $\delta = \omega_p - \omega_{p+hk} - \Delta$ and the atom-light detuning $\Delta = \epsilon_1 - \epsilon_0 - \omega$. Fig. 2 shows the eigenfrequencies with the gap $\Sigma = \sqrt{\delta^2 + \Omega^2}$. The energy structure indicates spin-orbit coupling of the neutral atom [12]. The EIW occurs around the points of energy degenerate, $p = -hk$ for $\Delta = 0$ and $p = 0$ for $\Delta = -\omega_p$ as illustrated in Fig. 2 (a) and (b). The area of EIW is also significant for the realization of artificial gauge field [16] and topological chiral edge states in cold atomic systems [17].

The averaged momentum of the atom wave packet can be calculated through the formula $\langle p(t)\rangle = \langle \psi(t)|p|\psi(t)\rangle$. From the function of momentum $p(t)$ we can obtain displacement of the atom $\langle x(t)\rangle = \langle x(0)\rangle + \int_0^t \langle v(t)\rangle dt$. 

In the strong coupling regime $\Omega \gg \delta$, we have $\Sigma \approx \Omega$ where the EIW would appears as illustrated in Fig. 2. In this regime, the displacement of the atom wave packet has the following simple form

$$\langle x(t)\rangle = \langle x(0)\rangle + \frac{p_c}{M}t + \frac{C_0^2 - C_1^2}{2M}(t - \frac{\sin(\Omega t)}{\Omega}).$$

Eq. (2) describes the coherent walking of single atoms [6] along the $x$ direction. Then, from the formula of atom wave packet displacement, velocity of the atom in the $x$ direction can be achieved as

$$\langle v(t)\rangle = \frac{p_c}{M} + \frac{C_0^2 - C_1^2}{2M}\frac{hk}{\Omega} \left(1 - \cos(\Omega t)\right).$$

It is obvious that displacement and velocity of the atom is changing periodically with the time periodicity $T = \frac{2\pi}{\Omega}$. The averaged velocity in a periodic time $\bar{v} = \frac{1}{T} \int_0^T \langle v(t)\rangle dt$ is

$$\bar{v} = \frac{p_c}{M} + \frac{C_0^2 - C_1^2}{2M}\frac{hk}{\Omega}.$$

Considering the experimental set up in Fig. 1 (a), initial velocity in $x$ coordinate can be zero, $p_c = 0$. In addition, the input atoms are assumed to be in the ground state $C_0 = 1$ now. It results the simple relation between atom velocity and its mass-wave length product as

$$\bar{v} = \frac{\hbar}{2Ma}.$$

where $\hbar$ is the Plank constant. Eq. (3) reveals that as soon as the product of atom masses $M_i$ and a resonant wave lengths $\lambda_i$ of corresponding atoms are different in a mixed atomic gas, $M_i\lambda_i \neq M_j\lambda_j$ for $i \neq j$, these chemical elements could be separated physically in principle.
TABLE I: Atom samples ($u = 1.67 \times 10^{-27}$ kg)

| Element | Mass $M$ (u) | Transition $|0\rangle \rightarrow |1\rangle$ | Wavelength $\lambda$ (nm) | Speed $\frac{h}{2\pi M}$ (m/s) |
|---------|-------------|---------------------------------|-------------------|------------------|
| $^7$Li  | 7.016004    | $2s^2S_{1/2} - 2p^2P_{1/2}^0$  | 670.7926          | 0.042153         |
| $^{12}$C | 12.000000   | $2s^2p^2P_{1/2} - 2s^2p_0^2(3P)'$ | 165.6928          | 0.099775         |
| $^{20}$Ne | 19.992435   | $2p^6 1S_0 - 2p^5(3P_{1/2})_0^0$ | 626.8232          | 0.01583          |
| $^{24}$Mg | 23.985042   | $3s^2 1S_0 - 3s 3p^1 P_1^0$     | 285.21251         | 0.02900          |
| $^{25}$Mg | 24.985837   | $3s^2 1S_0 - 3s 3p^1 P_1^0$     | 285.21251         | 0.027830         |
| $^{26}$Mg | 25.982930   | $3s^2 1S_0 - 3s 3p^1 P_1^0$     | 285.21251         | 0.02677          |
| $^{28}$Si | 27.976927   | $3s^2 3p^2 3P_0 - 3s^2 3p_0^4 3P_1^0$ | 251.4316          | 0.028202         |
| $^{40}$Ca | 39.962591   | $4s^2 1S_0 - 4s 4p 1P_1^0$      | 422.6277          | 0.011745         |
| $^{48}$Ti | 47.947947   | $3d^4 4s^2 a^5F_{2} - 3d^2(F)4s^4p(3P)^0 z^2D_1^0$ | 501.4186          | 0.008251         |
| $^{56}$Fe | 55.934939   | $3d^6 4s^2 a^5D_{4} - 3d^5(5D)4s4p(3P) z^2P_0$ | 248.32708         | 0.014282         |
| $^{59}$Co | 58.933198   | $3d^7 4s^2 a^5F_{9/2} - 4d^5(F)4s4p(3P)^0 z^2F_{9/2}^0$ | 352.6850          | 0.009544         |
| $^{69}$Ga | 68.925580   | $4s^4 4p 2P_{1/2}^0 - 4s^6 5s^2 S_{1/2}^0$ | 403.2984          | 0.007136         |
| $^{85}$Rb | 84.911794   | $5s 2S_{1/2} - 5p 2P_{3/2}^0$   | 780.027           | 0.022995         |
| $^{87}$Rb | 86.909187   | $5s 2S_{1/2} - 5p 2P_{3/2}^0$   | 780.027           | 0.020926         |
| $^{85}$Sr | 86.908884   | $5s^2 1S_0 - 5s 5p 1P_1^0$      | 460.733           | 0.004954         |
| $^{93}$Nb | 92.906377   | $4d^4(a^5D)5s^2 a^5D_{1/2} - 4d^3 5s(a^3P)5p y^6P_{3/2}^0$ | 353.530           | 0.006039         |
| $^{107}$Ag | 106.905092  | $4d^{10}(1S)5s^2 S_{1/2}^0 - 4d^{10}(1S)5p 2P_{3/2}^0$ | 328.0680          | 0.005656         |
| $^{114}$Cd | 113.903357  | $5s^2 2S_{1/2} - 5s 5p 1P_1^0$  | 228.8022          | 0.007122         |
| $^{115}$In | 114.903800  | $5p 2P_{1/2}^0 - 6s 2S_{1/2}^0$ | 410.1750          | 0.004209         |
| $^{133}$Cs | 132.905429  | $6s 2S_{1/2} - 6p 2P_{3/2}^0$   | 852.113           | 0.001751         |
| $^{153}$Eu | 152.921225  | $4f^7 6s^2 a^8S_{1/2}^0 - 4f^6(S)6s6p(1P)^0 y^6P_{3/2}^0$ | 466.188           | 0.002801         |
| $^{173}$Yb | 172.938208  | $4f^{14}(1S)6s^2 1S_0 - 4f^{14}(1S)6s6p 1P_1^0$ | 555.6466          | 0.0020645        |
| $^{197}$Au | 196.966543  | $5d^{10}6s^2 2S_{1/2} - 5d^{10}6p 2P_{1/2}^0$ | 267.5954          | 0.003763         |
| $^{238}$U | 238.050784  | $5f^{14}(4p)6d7s^2 Z_{1}^6 - 5f^{14}6d^2 7p 7S_{7/2}^0$ | 358.48774         | 0.0023247        |

Samples of chemical elements are listed in table I with related parameters. Every transition considered here is transition between the ground state $|0\rangle$ and an excited state $|1\rangle$. The wavelengths are corresponding to the resonant frequencies of these transitions, respectively. EIW speeds of these atoms are clearly different as shown in this table.

These speed difference gives rise to atom deflection as illustrated in Fig. 1 It is similar to the behavior of magnetic atoms in Stern-Gerlach experiment. The atom displacement in $x$ coordinate can be seen Fig. 3 (a), based on the parameters in Table I. Generally, the coherent walking of light atoms move faster and weight atoms move slower. It is good for separation of these atoms. However, due to there are more selections for the resonant wavelengths, some weight atoms can move faster than light atoms, such as $^{114}$Cd, light atoms. At the same time, some light atoms may move slower than weight atoms, such as $^{87}$Sr. The fact is benefit to the separation of atoms with similar masses, for example, $^{87}$Rb and $^{87}$Sr, $^{114}$Cd and $^{115}$In. Atoms plotted in Fig. 3 (a) are easily separated each other. The smallest speed difference comes from speed of $^{173}$Yb and speed of $^{238}$U. After 30μs, $^{238}$U atom exceeds $^{173}$Yb atom nearly 10 nm.

Commonly, isotopes are hardly separated. In the EIW based optical purification, isotopes can be distinguished only relying on their masses, since energy structure of isotopes are closed to be the same. Isotopes of light atoms are easier to be separated relatively. For example, the Magnesium isotopes shown in Fig. 3 (b). Their distances are nearly 50 nm at time 42 μs. Wight atoms such as Rubidium isotopes $^{85}$Rb and $^{87}$Rb leave each other about 50 nm after 500 μs as illustrated in Fig. 3 (c). The purification ability of the optical method can be further increased by extending coherent time of atoms. This advantage of this method can be seen from Fig. 3 (b) and (c).

A speed table of chemical elements are shown in Fig. 3 for given transition wavelengths. Speeds of atoms appear several clear ladders, from $^1$H to $^4$He, from $^7$Li to $^{19}$F, from $^{20}$Ne to $^{40}$Ar, from $^{89}$K to $^{84}$Kr, from $^{85}$Rb to $^{132}$Xe, from $^{133}$Cs to $^{219}$Rn and from $^{223}$Fr to $^{238}$U. It is very important for the separation of these chemical elements. Each speed of individual atom can be tuned by selecting other optical transitions.

This optical method should be developed into purification of molecular materials. Indeed, cooling and trapping of molecules has been realized recently by several research groups. It is known from these reports that masses and transition wavelengths of these cooled molecules are comparable to individual atoms. Furthermore, mass difference between different molecules are generally very large.
FIG. 3: (Color on line) (a) EIW displacements of different atom samples versus time. (b) EIW displacements of different Magnesium isotopes. (c) EIW displacements of different Rubidium isotopes.

FIG. 4: Velocity-table of chemical elements for given transition wavelengths. Corresponding wavelength with unit nm is written above each element. The inset is total data bars shown below.

In conclusions, we proposed a quantum mechanical method for precise purification of materials based on electromagnetically induced waking. A clear advantage of this method is that the separation ability is not only determined on difference of atom masses but also determined on difference of optical transition wavelengths. Therefore, all chemical elements and related isotopes can be separated physically with this configuration in principle. However, weight atoms and weight isotopes are still relatively hard to be separated in fact. Fortunately, there is another significant parameter in EIW that the atom coherent time. As soon as the atom coherent time is long enough, the hardly separable problems should be solved. This method could be mainly used to purify mixed materials which are in the state of fluid or gaseous. In most of times, low temperature is necessary.
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