A model of optical trapping cold atoms using a metallic nano wire with surface plasmon effect

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Abstract. In this work, we construct a new model of optical trapping cold atoms with a metallic nano wire by using surface plasmon effect generated by strong field of laser beams. Using the skin effect, we send a strong oscillated electromagnetic field through the surface of a metallic nano wire. The local field generated by evanescent effect creates an effective attractive potential near the surface of metallic nano wires. The consideration of some possible boundary and frequency conditions might lead to non-trivial bound state solution for a cold atom. We discuss also the case of the laser reflection optical trap with shell-core design, and compare our model with another recent schemes of cold atom optical traps using optical fibers and carbon nanotubes.

1. Introduction
In the last twenty years the problem of surface plasmon and surface plasmon polariton become one of the hottest topics, attract great intention, and their investigation grow up very quickly in both theoretical and experimental sides due the very large potential and vast application in modern nano and bio technologies [1-23].

Recently, study properties of cold neutral trapped atoms have attracted much interest because of their significance in both fundamental research and potential technological applications. So far, the investigation of hybrid systems that integrate isolated atoms with solid devices has become a hot research subject in both atomic physics and nano-optics [24-31]. The crucial property of these devices is the ability of the designed system to trap and manipulate cold atoms near the surface of the device in a nanoscale region. To trap, guide, and manipulate cold atoms in a nanoscale region, several different methods have been proposed [24,26] in which metallic nanometer structures have been paid more attention due to the property of plasmon resonances and exhibiting surface plasmons (SPs). The trapping methods of neutral atoms are of interest in applications in many domains of physics. Cold and trapped radioactive atoms can be used in the fundamental symmetry experiments, including the experiments on nuclear $\beta$ -decay, atomic parity non conservation and the search for parity and time-reversal violating electric dipole moment. Trapping of ultracold atoms also gives us an opportunity to study the collisional processes in cold atomic samples. Trapped cold atoms can be used in the formation of cold molecules and in studies of quantum statistical effects in atomic ensembles at low temperatures, such as the Bose-Einstein condensation (BEC). Since the cold molecules trap lifetime was approximately half a second, so the production of cold molecules opens up new ways
of research in molecular spectroscopy. There are different schemes for trapping and storing cold
atoms [24-31] such as optical trapping using the forces of electric dipole interaction between
atoms and laser fields, magnetic trapping based on the use of the forces of magnetic dipole
interaction, mixed magneto-optical trapping using simultaneous interaction between atoms and
magnetic and laser fields, and also mixed gravito-optical and gravito-magnetic trapping.

In the previous works [28-31], we have shown that the neutral atoms and molecules can
be captured at temperature down to nano-Kelvin by an optical trap, based on the use of an
evanescent wave around a thin optical fiber, a single wall carbon nanotube (SWCNT) or other
nano structures.

In this work we study the optical trap using the surface plasmon effect. This scheme gives
strong effect on cold neutral atom, which need to be shown experimentally. Plasmon and plasmon
polaritons theories always are difficult to understand for numerous experimental physicists and
technicians, a simple model will be useful and needed.

2. Surface plasmon SP and surface plasmon polariton SPPs in cylindrical metallic
nanowires
Owing to the fact that the modified Drude model (MDM) is based on the Sommerfeld theory
of metal, Maxwells equations and Newtons theory can be used to deal with the interaction
between the free electrons in the metal and the penetrated electromagnetic fields (EM): under
the excitations of the penetrated fields, the free electrons will execute a collective motion. For
an single metal wire (SW), in particular a thin SW, subjected to the penetrated fields, the
uniformly distributed free electrons within the wire are re-arranged to form a bunch-like state.
On the other hand, due to the space charge effect, the electrons tend to return to their original
uniform spatial distribution. These processes are the general physical basis of the following
analyses.

When the axial symmetric mode ($TM_0$ mode) is excited (symmetric excitation) on the SW,
the free electrons in the metal can oscillate longitudinally only in the vicinity of the surface
of the wire, which is just the case of surface plasmon polariton (SPPs). So, the $TM_0$ mode
is always the surface propagating mode. Yet, when the wire is excited by an asymmetric
mode (asymmetric excitation), the natural uniformly distributed free electrons in the metal
are forced to change into electron bunches along the angular direction within the wire to match
the azimuthal variation of the penetrated fields; the electron bunches will execute spiral motion
along the wire by combining the longitudinal and transversal motions of the electrons. According
to the electrodynamics theory, the transversal rotation of the electron bunches will emit EM
radiation, which is just the physical mechanism of the radiation of the asymmetric mode.

The mechanism of the mode transformation for SPPs propagating along SW can be explored.
When an asymmetric mode is excited on a very thin metal wire, the field penetration into the wire
is very strong. The free electrons are forced to change their original uniform spatial distribution
state, and the distribution re-arrangement of free electrons occurs in the wire to form electron
bunches, which will also execute a special spiral motion along the wire. This motion causes the
asymmetric mode to rapidly disappear through radiation. On the other hand, the variation of
the spatial distribution of the electrons will result in a strong space charge force, which leads to
a reverse trend for the re-arranged electron distribution returning to the original uniform state
gradually.

To calculate the group velocity $d\omega = dk$ as a function of a metallic nano wire radius $R$, a
model consisting of a metallic cylinder with a dielectric constant $\epsilon_m$ surrounded by a dielectric
medium of dielectric constant $\epsilon_d$ was used (see the figure 1).

For the special case with TM mode ($H_z = 0$) and fundamental mode with no winding $m = 0$,
continuity of the remaining tangential components $E_z$ and $H_\phi$ at the boundary lead to the
equation for SPPs dispersion relations.
The surface plasmon propagation in this case is governed by the dispersion relation for the fundamental transverse magnetic mode, which is given by [16, 22]

\[ k^2 J_0 (k_{2\perp} R) - k^2_{1\perp} H_0' (k_{1\perp} R) = 0, \]

where \( k_i = \sqrt{\epsilon_i \omega / c} = \sqrt{k^2_{i\perp} + k^2_{i\parallel}} \) and \( J_m, H_m \) are Bessel and Hankel functions of the first kind, respectively. By numerically solving the above equation (1), we can compute the group velocity as a function of \( R \) for a given frequency \( \omega \) and given \( \epsilon_d, \epsilon_m \).

In the limit of \( k_{i\perp} = \sqrt{k^2_{i\perp} - k^2_{i\parallel}} \approx ik_{i\parallel} \) we have

\[ \epsilon_m / \epsilon_d = \frac{K_1 (k_{i\parallel} R)}{K_0 (k_{i\parallel} R)} \frac{I_0 (k_{i\parallel} R)}{I_1 (k_{i\parallel} R)}, \]

with \( K_m, I_m \) are modified Bessel and Hankel functions, respectively.

Taking the case of metal/vacuum interface \( \epsilon_d = 1 \), and using the relation \( \omega^2 = \omega^2_P (\epsilon_\infty - \epsilon_m) \), the SSP dispersion relation for metallic nano wires is

\[ \omega_{DW} (k_{\parallel}, R) = \omega_P \left\{ \epsilon_\infty - \frac{K_1 (k_{\parallel} R)}{K_0 (k_{\parallel} R)} \frac{I_0 (k_{\parallel} R)}{I_1 (k_{\parallel} R)} \right\}^{-1/2}, \]

here \( k_{\parallel} \) is the in-plane (parallel to metal/dielectric surface) part of the wave vector.

In the case of small radius nanowires \( k_{\parallel} R \leq 1 \) we obtain the dispersion relation for SPPs

\[ \omega_{DW} (k_{\parallel}, R) \approx \omega_P \left\{ \epsilon_\infty - \frac{2\epsilon_d}{a + ln (k_{\parallel} R)} \right\}^{-1/2}, \]

where \( a = \gamma_E - ln2, \gamma_E = 0.577 \) is the Euler’s constant.

Because in the case of plasmon-plariton the longitudinal-transversal splitting is zero \( \omega_{LT} = 0 \), so we can consider the dispersion relation (3, 4) also for \( k_{\perp} \) the off-plane (orthogonal to metal/dielectric surface) part of the wave vector. In the following parts of this work, we will omit the sub-index \( \parallel, \perp \) of the \( k \) wave vector.

3. Simple SPPs model for cylindrical metallic nanowires

In analogy the cases of exciton plariton and phonon polariton, we consider a model Hamiltonian in 2nd quantization form for surface plasmon polariton [23] in metallic nano wires.
\[ H = \sum_k H_k = \sum_k \left\{ \omega_{\gamma_k} a_k^+ a_k + \omega_{P1} b_k^+ b_k + g_k \left( a_k^+ b_k + b_k^+ a_k \right) \right\}, \quad (5) \]

with \( a_k(a_k^+) \) and \( b_k(b_k^+) \) are the annihilation (and creation) photon and plasmon operators correspondingly with momentum \( k \), \( \omega_{P1} \) is the surface plasmon energy with \( m = 0 \), the fundamental model will be denote by the symbol 1, and \( \omega_{\gamma_k} = ck/\sqrt{\epsilon_d} \) is the photon dispersion law.

We denote \( g_k \) the plasmon-photon transition vertex (or coupling constant), this vertex is absence in traditional plasmon theory \( g_{Bk} = 0 \) because the bulk plasmon is longitudinal excitation, while photon is transversal excitation. For the case of surface plasmons due to the existence of the boundary conditions that electromagnetic waves must be satisfied at the interface, the plasmon-photon transition vertex might not be zero, and being the main parameter of our theory.

We use the Bogoliubov transformation technique taken from theory of superconductivity for diagonalisation plasmon polariton Hamiltonian

\[ H_k = \sum_k \left\{ \Omega_{Uk} \gamma_{Uk}^+ \gamma_{Uk} + \Omega_{Lk} \gamma_{Lk}^+ \gamma_{Lk} \right\}, \quad (6) \]

where \( \gamma_{\nu k} \) (and \( \gamma_{\nu k}^+ \)) are the annihilation (and creation) operators of the surface plasmon polariton SPPs with momentum \( k \), and \( i \) is the branch number \( i = L = 1 \) for lower and \( i = U = 2 \) for upper branch.

The transformations with unita condition \( u_k^2 + v_k^2 = 1 \) are

\[ \gamma_{1k} = u_k a_k + v_k b_k, \quad \gamma_{2k} = -v_k a_k + u_k b_k. \quad (7) \]

Using the commutative relations for annihilation and creation operators \([a_k, a_k^+] = 1, b_k(b_k^+] = 1, [\gamma_{\nu k}, \gamma_{\nu k}^+] = 1\), and equal zero for others, by standard calculation we obtain the surface plasmon polariton SPPs dispersion relations

\[ \Omega_{\nu k} (R) = \frac{1}{2} \left\{ [\omega_{\nu k} \pm \omega_{P1} (R)] - \sqrt{[\omega_{\nu k} - \omega_{P1} (R)]^2 + 4g_k^2} \right\}. \quad (8) \]

Note that in the case of planar geometry, the upper branch is lying in the energy gap where the damping is too high so only the lower branch exist, while in the case of metallic nano wires both SPPs branches could be exist.

We take the Dispersion relations of the lowest energy SPPs modes on the silver nanowire of the metallic nanowires in the form

\[ g_{Wk}^2 (R) = [\omega_{k+} - \omega_{DW} (k, R)]^2 - \omega_{k-}^2, \quad (9) \]

where

\[ \omega_{k\pm} = \frac{1}{2} (\omega_{P1} \pm \omega_{\gamma_k}), \quad (10) \]

and \( \omega_{DW} (k, R) \) is the Drude-like SPPs dispersion relation

\[ \omega_{DW} (k, R) = \left\{ \omega_{\gamma_k}^2 + \omega_{P1}^2 (R) - \sqrt{\omega_{\gamma_k}^4 + \omega_{P1}^4 (R)} \right\}^{1/2}. \quad (11) \]

Note here our plasmon-photon effective coupling constant is well defined via \( \omega_{\gamma_k} \) and \( \omega_{P1} (R) \).

The value of the plasmon-photon coupling constant \( g_k \) depends on wave vector \( k \) at the metal/vacuum interface of metallic nanowires (\( \epsilon_d = 1 \)) is plotted in the figure 2.
Figure 2. The value of the plasmon-photon coupling constant $g_k$ depends on wave vector $k$ at the metal/vacuum interface of metallic nanowires.

Figure 3. The calculated from Eqs. (8, 9) dispersion relation $\Omega$ and plasmon-photon coupling constant $g_k$ of the lowest energy SPPs modes with experimental data (blue dots).

The bottle neck region $k \simeq k_p$ is most important for all polariton problems, from this picture we can approximately take $g_{P1} = g_{k=k_p} \simeq 0.3\omega_{P1}$ for simple calculation and estimation.

For comparison, we take the case of Ag cylindrical nano wires with the data set $\omega_{P1} = 1370$ THz, $R = 100$ nm, $\epsilon_\infty = 2.9$. The calculated from Eqs. (8, 9) dispersion relation $\Omega = \Omega_L(k)$ and plasmon-photon coupling constant $g_k$ of the lowest energy SPP modes with experimental data (blue dots) are presented in the figure 3. The plamon energy 1370 THz was shown also for guidance. We can see the good agreement between theoretical and experimental results.

As mentioned above we can approximately take $g_{P1} \simeq 0.3\omega_{P1} = 450$ THz for simple estimations.

4. Cold atom surface plasmon polariton trapp with cylindrical metallic nanowires

The schema of our model is an analogy of the optical trap model [24-31], but the optical fiber is replaced by a metallic nano wire with radius $R$.

For a clear comparison with the optical trap model using a silica fiber [29] and metallic nano wire with evanescent effect, we use evanescent wave filed by plasmon surface effects induced, the wave decays away from the metallic nano wire surface producing an attractive potential for the neutral atom. The atom needs to be kept away from the metallic nano wire for a stable trapping, the waveguide possibility of metallic nano wire is observed experimentally [21]. We assume that the input light fields are circularly polarized to produce the cylindrically symmetric optical potential. The optical potential of the atom is cylindrically symmetric, that depends on the radial distance $r$ from the atom to the carbon nanotube axis $Z$, but not on two other cylindrical coordinates $\varphi$ and $z$. The optical field generates an evanescent wave around the...
metallic nano wire to capture cold atoms. Assume that the time scale of atomic motion is much slower than the beating period of the light field, that is, the inverse of their frequency difference. The component $L_z$ of the angular momentum of the atom is conserved, $L_z = m\hbar$ in the eigenstate, where $m$ is an integer, called the rotational quantum number. The centrifugal potential of the atom is repulsive and can be written as [24, 25]

$$U_{cp} = \hbar^2 (m^2 - 1/4) / 2\mu^2,$$

where $\mu$ is the atomic mass. A circularly polarized light was sent through the wire to produce the cylindrically symmetric potential $U$. The radial motion of the atom can be treated as the one-dimensional motion of a particle in the effective potential

$$U_{eff} = U_{cp} + U.$$

A circularly polarized light was sent through the fiber to produce the cylindrically symmetric potential $U$. The optical field generates an evanescent wave around the metallic nano wire. The metallic nano wire mode characteristic is determined by the radius $R$ and light wavelength $\lambda$. The parameter $q = 1/\Lambda$ is the inverse of the characteristic decay length $\Lambda$ of the evanescent-wave field. The modified Bessel function $K_0(qr)$ is used to describe the spatial dependence of the amplitude of the field outside the carbon nanotube in the linear-polarization approximation. $G$ is the coupling constant for the interaction between the evanescent wave and the atom, then $U = -GK_0^2(qr)$ is the optical potential outside the metallic nano wire. The effective potential for the radial motion of the atom can be written as

$$U_{eff} = \theta_{rec} \left[ \frac{m^2 - 1/4}{k^2 r^2} - \frac{g}{k^2} K_0^2(qr) \right],$$

where $\theta_{rec} = (\hbar k)^2 / 2\mu$ is the recoil energy, $g = G/\theta_{rec}$ is the normalized coupling parameter and $k$ is the wave vector of the field. The potential $U$ is attractive, opposite to the centrifugal potential $U_{cp}$. The atom can have a stable bound state only if $U_{eff}$ has a local minimum at distance $r = r_m$ and allow at least one bound state exist.

The Schrodinger equation of a cold atom around the cylindrical metallic nanowire is written in the cylindrical system of coordinates $(r, \varphi, z)$ is

$$\left[ -\frac{\hbar^2}{2\mu} \nabla^2 + U_{eff} \right] \psi(r, \varphi, z) = E\psi(r, \varphi, z),$$

where $E$ is the energy of atom in the optical potential, the wave functions are taken in the form $\psi(r, \varphi, z) = \frac{1}{\sqrt{r}} R(r)e^{im\varphi}e^{ikz}$. The Schrodinger equation for radial motion of the atom in the presence of effective optical potential $U_{eff}(r)$ is

$$\frac{d^2 R}{dr^2} + \frac{2\mu}{\hbar^2} \theta_{rec} \left[ \varepsilon - \left( \frac{m^2 - 1/4}{k^2 r^2} - \frac{g}{k^2} K_0^2(qr) \right) \right] R = 0,$$

with $\varepsilon = E/\theta_{rec}$.

The Schrodinger equation (16) can be solved numerically only. In the previous works [28-31], we replaced the “exact” potential $U_{eff}$ by a Morse-like simple effective potential. The set of parameters of this Morse-like effective potential was found by fitting with the “exact” potential or experimental data. With the Morse-like effective potential, the new Schrodinger equation now can be solved analytically. By that the lowest bound energy (ground state) is obtained and the efficiency of trap was estimated.
In the case of surface plasmon mechanism, the normalized coupling parameter is too large that instead of Morse-like effective potential we choose the exponential effective potential

\[ V_{\text{eff}}(r) = -V_0 \exp\left(-\frac{r}{\delta}\right), \]  

where \( V_0 \) and \( \delta \) are parameters of our model. We take \( V_0 = g_P \approx 0.3 \omega_P \), and \( \delta \) is the plasmon penetration length generated by evanescence field of surface plasmon in vacuum or air

\[ \delta(\omega) = \frac{1}{|k_d|} = \frac{c}{\omega} \sqrt{\frac{|\epsilon_m + \epsilon_d|}{\epsilon_d^2}}, \]  

(18)

The binding energy (ground state) of the Schrodinger equation with the exponential potential (17) is

\[ E = -\frac{\hbar^2}{8\mu \delta^2} \beta^2, \]  

(19)

where \( \beta \) is defined by the equation

\[ J_\beta\left(\frac{2\delta}{\hbar} \sqrt{2\mu V_0}\right) = 0, \]  

(20)

and \( J_\beta \) is the Bessel function. Because the argument of the Bessel function is too large \( \frac{2\delta}{\hbar} \sqrt{2\mu V_0} \gg 1 \), so in practical the equation (20) is not easy to solve.

For estimation we take the \( V \)-potential

\[ V(r) = ar - b, \]  

(21)

with the conditions that the two potential have the same deep and the same average efficiency

\[ V(0) = V_{\text{eff}}(0), \quad \int_0^{r_{\text{max}}} V(r) \, dr = \int_0^\infty V_{\text{eff}}(r) \, dr, \]  

(22)

where \( r_{\text{max}} = b/a \). From these conditions we get \( b = V_0 = g_P \), and \( a = V_0^2 / (2\delta) = g_P / (2\delta) \). The new effective \( V \)-potential equals

\[ V(r) = \frac{g_P}{2\delta} r - g_P. \]  

(23)

The values of \( V \)-potential (yellow) and exponent potential (blue) are presented in the figure 4.

The energy spectra of Schrodinger equation with the \( V \)-potential can be obtained exactly by WKB method. The basic idea of the old quantum theory is that the motion in an atomic system is quantized, or discrete. The system obeys classical mechanics except that not every motion is allowed, only those motions which obey the old quantum condition

\[ \int_{r_1}^{r_2} p \, dr = nh, \]  

(24)

where \( \hbar \) is the quantum constant, \( r_1, r_2 \) are the turning points derived from equation \( H(p, r) = E \). For \( V \)-potential \( r_1 = 0, r_2 = b/a = \delta \), the quantum condition reads

\[ \int_0^\delta dr \sqrt{2\mu \left(E - \frac{g_P}{2\delta} r + g_P \right)} = nh, \]  

(25)

so
Figure 4. The values of $V$-potential (yellow) and exponent potential (blue)

\[
\frac{4}{3} \sqrt{2\mu} \frac{(E + g_P)^{3/2}}{(g_P/2\delta)} = n\hbar = n2\pi\hbar,
\]

which determines the energy levels

\[
E_n = -g_P + \left(\frac{3\pi\hbar g_P}{4\delta \sqrt{2\mu}}\right)^{2/3} n^{2/3},
\]

and the lowest energy level (ground state)

\[
E_1 = -g_P + \left(\frac{3\pi\hbar g_P}{4\delta \sqrt{2\mu}}\right)^{2/3}.
\]

The condition exist at least one bound state reads $E_1 < 0$, or $g_P > (3\pi\hbar g_P/4\delta \sqrt{2\mu})^{2/3}$, or

\[
\delta \sqrt{g_P} > \frac{3\pi\hbar}{4\sqrt{2\mu}}.
\]

Now we estimate our obtained results. For estimation we take Ag nanowire with $\omega_{P1} = 1370$ THz, $R = 100$ nm, $\epsilon_\infty = 2.9$, $g_P = g_{P1} \approx 0.3\omega_{P1} = 450$ THz, $\delta \approx 50$ nm, the cold atoms are cerium Ce atoms with $\mu = 140 M_0$, $M_0 \approx 1$ GeV is the neutron mass. We use the thermal QED unit system with $\hbar = c = k_B = 1$, in which all physical values have to converted to eV energy unit, $\omega_{P1} = 5.6$ eV, $g_P \approx 0.3\omega_{P1} = 1.7$ eV, $\delta = 7.4$ eV, $\mu = 1.4 \times 10^{11}$eV, $k \approx 2$ eV (UV and optical range). We got that the condition (29) always satisfied, a bound state always exit, the SPPs mechanism trap factor $g_P/\theta_{rec} \approx 1.5 \times 10^{10}$. Compare with non-SPPs trap mechanism factors $G/\theta_{rec} \sim 6 \times 10^{3}$[24-31], the SPPs enhancement factor in trapping efficiency $\eta = g_P/G \sim 10^6$ in agreeing with the very large enhancement factors in another phenomena with SPPs mechanism, such as SERS [1-3], GFRET [18], ... The bounding energy of the the SPPs trap mechanism is $E_B = -E_1 \approx g_P = 1.7$ eV, which corresponds to the temperature $T_{SPPs} \sim 2 \times 10^4$ K, comparing with traditional optical trap temperature $T_i \sim 1$ mK [24-31], the SPPs enhancement factor in temperature is $\sim 10^7$. Trap with the SPPs mechanism, the “cold” condition of atoms seems not to needed anymore.

4. Conclusion

We have shown that the neutral cold atoms moving near a metallic nano wire can be captured by surface plasmon effect. The main idea is the considering a design model of trapping cold atoms with a metallic nano wire, by that the both two trapping effects can be used: optical
evanescence and plasmon effects. Using surface plasmon effect, there are more choices of light sources and the estimated trapping efficiency could be in 6-7 orders stronger than efficiency of traditional trap models without plasmon effect. Since a metallic nano wire offer the possibility of engineering evanescent fields and surface plasmon effect., the system can be used to store, move, and manipulate cold atoms in a controlled manner. The our proposed model might be useful in practical design of cold atom SPPs trap with metallic nanowires.

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