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All-optical nanotraps for atoms atop flat metamaterial lenses: a theoretical study

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Abstract

We propose a novel setup for optically trapping neutral atoms based upon the focusing properties of metamaterials. The optical trap is created at the focal point of an inverted-opal crystal when the latter is illuminated by a localized light source. The trap is located away from the surface of the inverted-opal lens, rendering the Casimir–Polder attraction exerted by the lens on the atom negligible. The key properties of the proposed optical trap are its subwavelength dimensions, the tunability of the trapping frequency, the facile translation of the trap without moving the lens, and the potential for creating an array of traps. We also study the ground state of a cesium Bose–Einstein condensate formed within the proposed trap by solving the corresponding time-independent Gross–Pitaevskii equation.

(Some figures in this article are in colour only in the electronic version)

1. Introduction

Atom trapping through purely optical means has been promoted as a more versatile and robust technique over magnetic trapping since optical potentials allow atoms in all hyperfine states to be confined whilst enabling, at the same time, the application of Feshbach resonances in the trapped atoms [1, 2]. A significant attention has been paid to dielectric structures which produce an optical potential when illuminated by an external source [3, 4]. The main challenge in trapping atoms with these structures and subsequently in the realization of corresponding atom chips is to overcome the strong Casimir-Polder (CP) potential exerted on the trapped atoms by the structure. The simplest approach is to confine the atom in the evanescent field near the surface of high-refractiveindex material, under (oblique) plane wave illumination. In this case, however, the decay length of the surface state in the direction normal to the interface is large and fixed by the dielectric constant of the chosen high-index material; this obstructs the emergence of a minimum of the total potential (optical + CP + gravitational). In a recent work, an alternative approach has been proposed, where the atomic gas is confined within a surface state of a truncated one-dimensional (1D) photonic crystal [5]; in this case, the free-space decay length of the surface state can be tuned to a desired value by altering the geometric characteristics of the photonic crystal.

In this work we propose a three-dimensional (3D) alloptical trap for neutral atoms which operates similarly to the optical tweezers. The optical potential is created at the focal point generated from the illumination by a localized source of a flat metamaterial lens [6]. The metamaterial is a Si-inverted opal (SiIO), which can create the image of a light source due to the existence of left-handed frequency bands, in which case negative refraction (NR) and focusing phenomena occur [7]. Since the dielectric function of Si remains constant within a wide spectral range, the left-handed bands of the metamaterial lens can be properly tuned by varying the period of the SiIO in order to match the desired atomic transition responsible for the trapping. The focal point providing the optical trap can be formed at a distance over one 1 μ m away from the surface of the metamaterial; this renders the CP potential negligible. In this case, the conditions for the formation of a potential minimum are less restrictive as only the gravity adds to the optical potential. The proposed all-optical atomic trap atop a flat metamaterial lens exhibits several other advantages: the absence of an optical axis, the translational invariance of the trap and the potential to create multiple traps [6]. The paper is organized as follows: section 2 presents the basic formalism for the calculation of the optical and CP potentials, which, together with gravity, provide the total potential experienced by the trapped atom. Section 3 applies the formalism to the case where an SiIO metamaterial lens is used to trap a Cs atom. Section 4 presents a discussion and the future outlook of the proposed trap while section 5 concludes the paper.

2. Theory

2.1. Optical potential

The lens producing the image trap is a finite slab of a metamaterial consisting of a number of planes of spheres with the same 2D periodicity. In order to probe the imaging properties of such a structure, we consider the electric field emitted by a localized source. The latter is written as a series of outgoing spherical waves [8],

$$\mathbf{E}(\mathbf{r}) = \sum_{l=1}^{\infty} \sum_{m=-l}^{l} \left\{ a_{Hlm} h_l^+(qr) \mathbf{X}_{lm}(\hat{\mathbf{r}}) + a_{Elm} \frac{\mathbf{i}}{q} \nabla \times [h_l^+(qr) \mathbf{X}_{lm}(\hat{\mathbf{r}})] \right\},$$
(1)

 $\mathbf{X}_{lm}(\hat{\mathbf{r}})$ are the so-called vector spherical harmonics [8] and h_l^+ are the spherical Hankel functions of order *l*. The wavenumber is $q = \omega/c$, where $c = 1/\sqrt{\mu\epsilon\mu_0\epsilon_0} = c_0/\sqrt{\mu\epsilon}$ is the velocity of light in the medium surrounding the source.

Since we wish to study the transmission of the above field through a slab of a number of periodic planes of spheres, it is advantageous to transform the field of equation (1) to a basis of plane waves consistent with the 2D periodicity of the planes of spheres. If the source is placed to the left of the slab (see the calculation setup in figure 2), the field radiated to the right and incident on the slab is written as (assuming the center of coordinates to be located at the localized source) [9]

$$\mathbf{E}^{\text{inc+}}(\mathbf{r}) = \frac{1}{S_0} \int \int_{\text{SBZ}} d^2 \mathbf{k}_{\parallel} \sum_{\mathbf{g}} \mathbf{E}_{\mathbf{g}}^{\text{inc+}}(\mathbf{k}_{\parallel}) \exp(i\mathbf{K}_{\mathbf{g}}^+ \cdot \mathbf{r}) \quad (2)$$

with

$$E_{\mathbf{g};i}^{\mathrm{inc+}}(\mathbf{k}_{\parallel}) = \sum_{l=1}^{\infty} \sum_{m=-l}^{l} \sum_{P=E,H} \Delta_{Plm;i}(\mathbf{K}_{\mathbf{g}}^{+}) a_{Plm} \qquad (3)$$

where i = 1, 2 are the two independent polarizations (polar and azimuthal) which are normal to the wavevector [10–12]

$$\mathbf{K}_{\mathbf{g}}^{\pm} = (\mathbf{k}_{\parallel} + \mathbf{g}, \ \pm [q^2 - (\mathbf{k}_{\parallel} + \mathbf{g})^2]^{1/2}). \tag{4}$$

The vectors **g** denote the reciprocal-lattice vectors corresponding to the 2D periodic lattice of the plane of spheres and \mathbf{k}_{\parallel} is the reduced wavevector which lies within the surface Brillouin zone (SBZ) associated with the reciprocal lattice [10–12]. When $q^2 < (\mathbf{k}_{\parallel} + \mathbf{g})^2$, the wavevector of equation (4) defines an evanescent wave. The coefficients Δ_{Plm} are given elsewhere [12]. The incident field of equation (2) will be partly transmitted through the slab under study. The transmitted field will be given by

$$\mathbf{E}^{\text{tr+}}(\mathbf{r}) = \frac{1}{S_0} \int \int_{\text{SBZ}} d^2 \mathbf{k}_{\parallel} \sum_{\mathbf{g}} \mathbf{E}_{\mathbf{g}}^{\text{tr+}}(\mathbf{k}_{\parallel}) \exp[i\mathbf{K}_{\mathbf{g}}^+ \cdot (\mathbf{r} - \mathbf{d})]$$
(5)

with

$$E_{\mathbf{g};i}^{\mathrm{tr}+}(\mathbf{k}_{\parallel}) = \sum_{\mathbf{g}',i'} T_{\mathbf{g}i;\mathbf{g}'i'} E_{\mathbf{g}'i'}^{\mathrm{inc}+}(\mathbf{k}_{\parallel}).$$
(6)

d is a vector joining the source to the image. The transmission matrix $T_{g_i;g'i'}$ appearing in equation (6) is calculated within the framework of the layer-multiple-scattering method, which is an efficient computational method for the study of the EM response of three-dimensional photonic structures consisting of non-overlapping spheres [10-12] and axisymmetric nonspherical particles [13]. The layer-multiple-scattering method is ideally suited for the calculation of the transmission, reflection and absorption coefficients of an electromagnetic (EM) wave incident on a composite slab consisting of a number of layers which can be either planes of non-overlapping particles with the same 2D periodicity or homogeneous plates. For each plane of particles, the method calculates the full multipole expansion of the total multiply scattered wave field and deduces the corresponding transmission and reflection matrices in the plane wave basis. The transmission and reflection matrices of the composite slab are evaluated from those of the constituent layers.

The calculation of the incident (equation (2)) as well as the transmitted field (equation (5)) requires a numerical integration over the entire SBZ. In the case of the SiIO examined below, the spheres in each plane occupy the sites of a square lattice and, therefore, the SBZ is also a square. The SBZ integration of equations (2) and (5) is performed by progressively subdividing the SBZ into smaller and smaller squares, within which a nine-point integration formula [14] is very efficient. Using this formula we managed excellent convergence with a total of 73 728 points in the SBZ. Also, the inclusion of 37 reciprocal-lattice **g**-vectors along with an angular-momentum cutoff $l_{max} = 7$ provided converged results.

From equations (5) and (6) we obtain the electric-field intensity $I(\mathbf{r}) = \frac{1}{2}\epsilon_0 |\mathbf{E}(\mathbf{r})|^2$ on the right side of the structure. Having found the distribution of $I(\mathbf{r})$, the optical-dipole potential for a given atomic transition is given by [5]

$$U_{\rm opt} = \beta_{\rm s} \frac{\hbar \Gamma^2}{8\delta} \frac{I(\mathbf{r})}{I_{\rm sat}}$$
(7)

where $\beta_s = 2/3$ and I_{sat} the saturation intensity [5]. Γ is the linewidth of the atomic transition and δ is the detuning of the incident radiation frequency from the transition frequency ω_0 (these parameters are explained in figure 1).

2.2. Casimir–Polder potential

The CP potential is given by [15]

$$U_{\rm CP} = 2\hbar\mu_0 \int_0^\infty du \, u^2 \alpha(iu) \sum_i G_{ii}(\mathbf{r}, \mathbf{r}; iu) \qquad (8)$$

where α is the atomic ground-state polarizability and $G_{ii'}^{EE}$ the electric-field component of the EM Green's tensor associated with the trapping structure. For a finite slab of a metamaterial,



Figure 1. Parameters concerning an atomic transition between states $|1\rangle$ and $|2\rangle$.

the Green's tensor is given by

$$G_{ii'}^{EE}(\mathbf{r}, \mathbf{r}; \omega) = g_{ii'}^{EE}(\mathbf{r}, \mathbf{r}; \omega) - \frac{l}{8\pi^2} \int \int_{SBZ} d^2 \mathbf{k}_{\parallel} \times \sum_{\mathbf{g}} \frac{1}{c^2 K_{\mathbf{g};z}^+} v_{\mathbf{g}\mathbf{k}_{\parallel};i}(\mathbf{r}) \exp(-i\mathbf{K}_{\mathbf{g}}^+ \cdot \mathbf{r}) \hat{\mathbf{e}}_{1;i'}(\mathbf{K}_{\mathbf{g}}^+)$$
(9)

with

$$v_{\mathbf{g}\mathbf{k}_{\parallel};i}(\mathbf{r}) = \sum_{\mathbf{g}'} R_{1\mathbf{g}';1\mathbf{g}} \exp(-\mathrm{i}\mathbf{K}_{\mathbf{g}'}^{-} \cdot \mathbf{r}) \hat{\mathbf{e}}_{1;i}(\mathbf{K}_{\mathbf{g}'}^{-}).$$
(10)

 $g_{ii'}^{EE}$ is the free-space Green's tensor and $\hat{\mathbf{e}}_{1;i}(\mathbf{K}_{\mathbf{g}}^{\pm})$ the polar unit vector normal to $\mathbf{K}_{\mathbf{g}}^{\pm}$. $R_{1\mathbf{g}';1\mathbf{g}}$ is the reflection matrix which provides the sum (over the **g**) of reflected beams generated by the incidence of the plane wave from the left of the slab [11, 12]. We note that the above expressions (equations (9) and (10)) are derived from the transverse part of the general classical wave Green's tensor [16].

2.3. Ground state of a Bose–Einstein condensate

For a thorough study of the trapping properties of the proposed setup, we need to calculate the ground-state properties of a Bose–Einstein condensate (BEC) formed within the trap. We consider the case of a BEC in a dilute atomic gas, in which case the Gross–Pitaevskii equation (GPE) [17, 18] applies

$$\left(\frac{-\hbar^2}{2m}\nabla^2 + U_{\text{trap}} + \frac{4\pi\hbar^2 a_{\text{sc}}N}{m}|\psi(\mathbf{r})|^2\right)\psi(\mathbf{r}) = \mu_c\psi(\mathbf{r}),\tag{11}$$

where $\psi(\mathbf{r})$ is the BEC wavefunction, U_{trap} is the total (optical + CP + gravitational) trapping potential, a_{sc} is the swave scattering length characterizing the two-body interaction between the atoms, N is the total number of atoms in the condensate, and μ_{c} the chemical potential. Equation (11) is solved by employing the basis-set expansion technique and corresponding programming code of [19]. Based on this technique, the trapping potential is approximated by a harmonic potential around one of its minima. In this case, the condensate wavefunction $\psi(\mathbf{r})$ is expanded in terms of either simple-harmonic-oscillator orbitals or Thomas–Fermi orbitals and equation (11) is solved self-consistently until convergence is reached. The solution of equation (11), apart from the BEC wavefunction $\psi(\mathbf{r})$ of the ground state, also provides the total energy per atom.



Figure 2. Setup of the all-optical atom trap.

3. Results

The setup of the proposed optical trap is shown in figure 2. It consists of finite slab of SiIO and a localized light source. An SiIO is a 3D photonic crystal made from air bubbles in Si, in an fcc-lattice configuration [20]. Originally, SiIOs were introduced as artificial materials with absolute photonic band gap [21]; however, as has been shown recently, the same structure can also act as a metamaterial exhibiting NR and, subsequently, focusing properties [7]. This means that an SiIO forms the image of a localized source when the latter emits radiation at a frequency belonging to a NR frequency band. The image of the source corresponds to a local maximum of the electric-field intensity which can be used as an optical trap. As a localized source one can use, for example, a quantum dot or a fluorescent molecule. However, one has to match the NR frequency band of the SiIO with a given atomic transition. This requires a certain amount of tunable response and operation of the proposed optical trap. Due to the almost constant value of the Si dielectric function within the frequency spectrum under study (infrared regime), the frequency band structure of the SiIO can be scaled according to the dimensions of the air spheres, allowing for an overlap between the NR band and the atomic-transition band. To be specific, we select a Cs atom using the D₂ resonant transition as in [5] with a frequency $\omega_0 =$ $2\pi \times 3.5 \times 10^{14}$ Hz. According to [7], optimal focusing due to NR occurs at a scaled frequency $\omega a/2\pi c = 0.603$ (a is the fcclattice constant of the SiIO). By assuming a red detuning of the order of $\delta = \omega - \omega_0 = -2\pi \times 0.1 \times 10^{14}$ Hz in the laser source, the lattice constant of the SiIO should be $a = 0.532 \ \mu m$ so that the D₂ transition falls within a NR band. As a localized source we have chosen a silver-coated SiO₂ nanosphere (metallic nanoshell). Namely, the scattered EM field from such a sphere simulates the EM field emitted by a dipole antenna of nanometer size due to the excitation of surface-plasmon (SP) resonances [22]. The emission frequency corresponds to one of the two SP resonances of the nanoshell, which can be properly tuned by varying the thickness of the silver shell [23]. If a Drude-type dielectric function is assumed for silver ($\epsilon(\omega)$ = $1 - \omega_p^2 / [\omega(\omega + i\gamma)]$ with $\hbar \omega_p = 3.8$ eV and $\gamma / \omega_p = 0.1$) then by choosing a shell thickness of 33.8 nm and a total nanosphere radius of 52 nm the particle-like SP of the silver-coated SiO₂ nanosphere matches the D₂ transition frequency ω_0 of Cs plus the detuning δ .

The source is placed at a distance a from the left side of finite slab of SiIO consisting of eight (100)-fcc planes of air



Figure 3. (Color online) Optical, gravitational, and total potentials (dotted, dashed and solid lines, respectively) for the case of Cs atoms as a function of the distance from the right surface of the SiIO lens along the direction (x, y) = (0, 0).

spheres in Si ($\epsilon = 12.25$). The source is placed right against an air sphere of the SiIO, i.e., so that a line connecting the centers of the nanoshell and an air sphere normal to the SiIO slab. As the frequency $\omega_0 + \delta$ falls within an NR frequency band of the SiIO (see above), the SiIO slab focuses the scattered field at an area at the right surface of the slab.

The D₂-transition linewidth is $\Gamma = 2\pi \times 5.3 \times 10^6$ Hz and the saturation intensity $I_{\text{sat}} = 1.1 \text{ mW cm}^{-2}$. In figure 3 we show the optical potential U_{opt} as a function of the distance from the right surface of the SiIO slab, along a direction normal to the slab (z-axis) and passing through the center of the source. We have chosen the maximum of the intensity $I(\mathbf{r})$ along this direction to be $I_0 = 10^5 \text{ mW cm}^{-2}$ (about 60% of the incident intensity) in order to obtain an optical potential of a few μ K. The minimum of the optical potential U_{opt} occurs at a distance 1.28 μ m from the surface of the SiIO slab. In figure 4 we show the distribution of the optical potential U_{opt} within the *xy*-plane, for the above distance. It is evident that there exists a prominent minimum of U_{opt} at (x, y) = (0, 0)with FWHM $w = 0.15 \ \mu m$, which is much smaller than both the wavelength ($\lambda = 2\pi c/(\omega_0 + \delta) = 0.882 \ \mu m$) and the lattice constant of the SiIO crystal ($a = 0.532 \ \mu m$). Along the z-direction (normal to the SiIO slab) the corresponding FWHM is about 0.32 μ m, which heralds the creation of a subwavelength trapping potential similar to that obtained with sophisticated macroscopic experimental setups [24]. Along with the main potential minimum there exist other satellite minima as a result of the inherent periodicity of the SiIO lens, which makes the focusing phenomenon imperfect [7]. The satellite minima, although shallower than the central one, can also act as optical traps, suggesting the possibility of having multiple traps with the proposed setup. It is worth noting that periodic (infinitely multiple) arrays of optical traps in a plane parallel to the surface (2D traps) can be created by simply illuminating a periodic structure with a plane wave [25]. In this case, however, a potential minimum in the z direction (normal to the surface) cannot occur either in the far- or in the nearfield regime. In the far-field regime one only has plane waves



Figure 4. Distribution of the optical potential for Cs atoms in the *xy* plane at a distance $1.28 \ \mu m$ from the SiIO lens, for the setup of figure 1. The potential is in units of μK .

whilst the in the near-field regime (close to the lens surface) the contribution of the CP potential to the total one is large and therefore renders the trap unsuitable for cold atoms.

In order to determine the actual trapping potential one must also take into account the CP (equation (8)) and the gravitational potential. The gravitational potential is given by $U_{\text{grav}} = mgr$, where m and g are the atomic mass and the gravitational acceleration, respectively, and r is the distance from the right surface of the SiIO lens. U_{grav} is also depicted in figure 3. By calculating the EM Green's tensor in the manner of equations (9) and (10) and substituting the atomic polarizability of Cs [26] it turns out that U_{CP} is of the order of a few nK when the distance between the atom and the trapping structure is of the order of 1 μ m and above. Therefore, for such distances the CP potential is negligible compared to the gravitational one and, in our case, to the optical potential for this order of radiation intensity. The total potential is thus determined as the sum of the optical and gravitational potentials as shown in figure 3. The position of the local minimum of the total potential is only slightly shifted relative to the minimum of the optical potential by the presence of the gravitational potential.

We note, however, that the actual depth of the trap corresponds to the ground state of Cs atom(s) within the total potential. Therefore, we solve the GPE (equation (11)) for a BEC of Cs atoms within the trapping potential of figures 3 and 4. The latter is approximated by a harmonic-oscillator potential of cylindrical symmetry around the global minimum, i.e.,

$$U_{\text{tot}} = \frac{1}{2}m(\omega_x^2 x^2 + \omega_y^2 y^2 + \omega_z^2 z^2)$$
(12)

with $\omega_x = \omega_y = 59.3$ Hz, $\omega_z = 23.75$ Hz. The s-wave scattering length is taken as $a_{sc} = 440a_0$ (a_0 is the Bohr radius), which is an optimal value for the formation of a Cs BEC [4]. In table 1 we show the BEC ground-state energy for different numbers of Cs atoms in the manner described in section 2.3. Obviously, in all cases the ground level lies very close to the bottom of the trapping potential. However, as the number of the trapped atoms increases, the repulsive interactions among them raise the energy of the ground state.

Table 1. The total energy per atom (in units of $\hbar \omega_x$) for different numbers of atoms.

Ν	Energy/N
1	1.200 5289
10	1.202 3934
100	1.220 5573
1 0 0 0	1.3697581
10000	2.115 4997

4. Discussion and outlook

As shown above, the occurrence of the minimum of the optical potential at a distance for which the CP potential is negligible allows for an easier manipulation of the optical trap: due to the monotonic change of the gravitational potential, the latter does not influence the position of the minimum of the total atomic potential. This might allow the movement of the trap by translating the source within the surface of the SiIO lens provided that the depth of the trap does not alter significantly (as in [6] where the movement of a trapped microparticle was demonstrated). This is difficult to achieve when the CP potential comes into play [5] since this type of potential is fixed by the composition and geometrical parameters of the trapping structure. For the same reason, the actual realization of proposals of optical traps created by the introduction of point defects in photonic crystals [27] is challenging since the trap is created close to the surface of the photonic crystal where the CP potential dominates. The same dominance of the CP potential is true in the case where the optical traps are created inside the photonic crystal [28].

One can now ask the question of whether it is possible to use infrared metamaterials with negative refractive index [29] instead of the SiIO. This type of NR metamaterials is subwavelength and so is the focal point created when they are illuminated by a localized source. In such a manner, one might be able to realize optical traps of a few nanometers size, enabling the realization of scalable quantum computers. However, such NR metamaterials are usually made from metallic components which are inherently lossy. In this case, the focal point is created very close to the surface, reviving the role of the CP potential. The same is true in the case of an optical trap generated near a microscope tip [30].

Another key property of the proposed atomic trap is its tunability: by proper choice of the lattice constant of the SiIO lens one can tune the working frequency of the trap to the relevant atomic transition. Another important property of the proposed optical trap is the absence of a particular optical axis. This fact allows the creation of multiple optical traps on the same SiIO lens by using more than one light sources. If a 2D lattice of the trap of figures 3 and 4 is desired, the light sources should be placed far apart in order to avoid interference effects from the scattering fields from all the sources. On the other hand, interference effects may be exploited to shape more efficiently the optical traps and, possibly, decrease their size.

We note that the avoidance of the CP potential as a result of the formation of the trap at a distance of more than one micron from the surface of the SiIO is in the opposite direction of the current trend in atom chips, where the traps are formed as close as possible to the surface. If the movement of the trap is not demanded, the proposed optical nanotrap can be used in conjunction with a typical magnetic trap such as a quadrupole trap formed by a pair of opposed Helmholtz coils [1]. In this case, the *z*-component of the magnetic field could also contribute to the neutralization of the CP potential, resulting in a total potential minimum closer to the SiIO surface.

Before the atoms are trapped in the proposed optical trap they need to be precooled by other means. This can be achieved, for example, by passing the atoms through a Zeeman slower [1] where their velocities become small enough to be trapped inside the proposed nanotrap. This is a common cooling technique used in trapping atoms with purely optical means.

A final note on the impact of the unavoidable fabrication imperfections on the proposed optical trap. In single-crystal opaline structures such as the SiIO lens considered here, the common types of lattice disorder are point defects and stacking faults [31]. The concentration of both types of disorder is too small to influence the optical properties of thin slabs of SiIO such as the eight-planes-thick slab considered here. Even the presence of one or two stacking faults does not influence much the transmission spectrum in the pass bands; stacking faults solely introduce defect states within the band gap of SiIO [32]. Typical samples of SiIO are polycrystalline in the sense that a cut of an SiIO contains domains corresponding to different crystallographic planes [33]. However, since the light sources used for creating the optical traps are much smaller than a typical domain size (around 50 μ m), polycrystallinity is not expected to pose a problem to trapping.

5. Conclusions

We have proposed a novel setup for trapping neutral atoms via purely optical means. The optical trapping potential is generated at the focal point of a metamaterial lens (slab of Si-inverted opal) which is probed by a localized source. By placing the source far enough from the metamaterial lens, the corresponding focal point occurs far from the lens, diminishing the contribution of the CP potential to the total atomic potential. This latter effect offers the possibility of translating the trap by simply moving the nanoshell. By proper tuning of the geometrical parameters of the metamaterial lens one can actually trap all kinds of atoms. The proposed alloptical trap can find application in various areas such as the control of chemical reactions by moving the participating atoms, in photoassociation of ultracold atoms and in nanoscale trapping of DNA [34]. Also, the prospect of having arrays of traps can find application in high-resolution detection of neutral particles and in ultracold atomic collision studies [34].

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