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Single atom in free space as a quantum aperture

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We calculate exact three-dimensional solutions of Maxwell equations corresponding to strongly focused light beams, and study their interaction with a single atom in free space. We show how the naive picture of the atom as an absorber with a size given by its radiative cross section $\sigma = 3\lambda^2/2\pi$ must be modified. The implications of these results for quantum-information-processing capabilities of trapped atoms are discussed.

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The resonant absorption cross section for a single two-state atom in free space driven by an electromagnetic field of wavelength λ is $\sigma = 3\lambda^2/2\pi$ [1]. Thus it seems reasonable to assume that a ''weak'' incident light beam focused onto an area $A \sim \sigma$ would experience a loss (as resonance fluorescence) comparable to the incident energy of the beam itself and would, for off-resonant excitation, suffer an appreciable phase shift. In terms of nonlinear properties, note that the saturation intensity for a two-state atom in free space is $I_s = \hbar\omega_a/2\sigma\tau$, where ω_a is the atomic transition frequency and $\tau = 1/\Gamma$ is the atomic lifetime. Hence, a single-photon pulse of duration $T \sim \tau$ should provide a saturating intensity and allow for the possibility of nonlinear absorption and dispersion in a *strong-focusing* geometry.

These considerations suggest that a single atom in free space could perform important tasks relevant to quantum-information processing, such as nonlinear entangling operations on single photons of different modes for the implementation of quantum logic, along the lines of Ref. [2], but now without the requirement of an optical cavity [3]. Further motivation on this front comes from the need to address small quantum systems individually, as for example in the ion-trap quantum computer [4,5] or in quantum communication protocols with trapped atoms in optical cavities [6,7]. Here, each ion (or atom) must be individually addressed by focusing a laser beam with resolution $\Delta x \gtrsim \lambda$ [8]. Interesting effects may also be expected with respect to the photon statistics of the scattered light in a regime of strong focusing, such as extremely large photon bunching [9]. Conversely, alterations of atomic radiative processes arising from excitation with squeezed and other forms of nonclassical light would be feasible as well [10]. Finally, questions of strong focusing become relevant for dipole-force traps of size λ for single atoms.

Against this backdrop of potential applications, we note that radiative interactions of single atoms with strongly focused light beams have received relatively little attention. Indeed, previous experiments have been restricted to a regime of *weak focusing* and resultingly small fractional changes in transmission [11–13], either because of large focal spot sizes $\sim 1000\lambda^2$ [12] or reduced oscillator strengths for molecular transitions [13]. On the theoretical front, we recall only Refs. [9] studying photon statistics by adopting a quasi-one-dimensional model.

In light of its fundamental importance, we report here the first complete three-dimensional (3D) calculations for the interaction of strongly focused light beams and single atoms in free space. Essential elements in this work are exact 3D vector solutions of Maxwell equations that represent beams of light focused by a strong spherical lens. As an application of our formalism, we calculate the scattered intensities and the intensity correlation function $g^{(2)}(0,\vec{r})$ as functions of angle for resonant excitation of a single atom with a strongly focused beam. We find an intriguing interplay between the *angular* properties of the scattered light and its *quantum-statistical* character (e.g., photon bunching and antibunching versus scattering angle), leading to the concept of a *quantum aperture*. Our results, in particular those corresponding to scattering in the forward direction, are compared to those of Ref. [9], and to similar calculations using 3D paraxial Gaussian beams [14], which we find do not always represent the actual situation with strongly focused light beams.

We start by constructing exact solutions of the Maxwell equations describing tightly focused beams (a detailed analysis is deferred to [15], see also [16]). An incoming (paraxial) beam with fixed circular polarization $\vec{\epsilon}_+ = (\hat{x} + i\hat{y})/\sqrt{2}$ and frequency ω propagates in the positive z direction and illuminates an ideal lens. The incoming beam is taken to be a lowest-order Gaussian beam with Rayleigh range $z_{\rm in}$ with $kz_{\rm in} \gg 1$, and is characterized by the dimensionless amplitude

$$\vec{F}_0 = \exp\left(-\frac{k\rho^2}{2z_{\rm in}}\right)\vec{\epsilon}_+ , \tag{1}$$

where ρ is the distance to the z axis and the wave vector $k = 2\pi/\lambda$. For simplicity the focal plane of the incoming beam and the plane of the lens are taken to coincide. After transforming this input field through the lens, the output field behind the lens is expanded in a complete set of modes $\vec{F}_\mu$ that are exact solutions of the source-free Maxwell equations adapted to the cylindrical symmetry of the problem, as constructed in [17]. The index μ is shorthand for the set of mode numbers $\mu = (k_t, m, s)$, with k_t the transverse momentum number $k_t = (k^2 - k_z^2)^{1/2}$, s the polarization index, and m the angular-momentum number [17]. For fixed k, the dimensionless mode functions $\vec{F}_\mu$ are normalized to

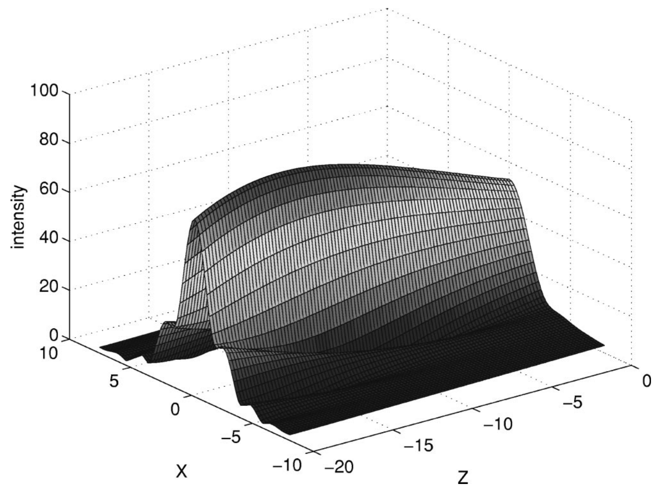

FIG. 1. Surface plot of the relative intensity $|\vec{F}_{\rm out}\cdot\vec{\epsilon}_+|^2$ of a strongly focused beam as a function of the dimensionless axial coordinate $Z\equiv(z-z_0)/\lambda$ and transverse coordinate $X\equiv x/\lambda$. The lens is located at $z=0$ and is characterized by $f=500\lambda$, with the incoming Gaussian beam having $z_{\rm in}/\lambda=6\times10^4$. This implies $z_0\approx500\lambda$ and $z_R\approx4.2\lambda$. For paraxial beams, the focal plane would be at $Z=0$.

$$\int_{z=\rm const}{\rm d}S\vec{F}_\mu^*\cdot\vec{F}_\nu=\delta(k_t-k_t')\delta_{mm'}\delta_{ss'}/(2\pi k_t). \qquad (2)$$

As for the field transformation by the lens, the action of a spherical lens is modeled by assuming that the field distribution of the incoming field is multiplied by a local phase factor $\exp(-ik\rho^2/2f)$, with f the focal length of the lens [18]. Thus, if in the plane of the lens, say $z=0$, the incoming beam is given by $\vec{F}_{\rm in}=\vec{F}_0$ as above, then the output field is given by

$$\vec{F}_{\rm out}(\vec{r})=\int {\rm d}k_t\sum_m\sum_s \kappa_\mu\vec{F}_\mu(\vec{r}), \qquad (3)$$

where for the particular choice of $\vec{F}_0$, κ_μ is [15]

$$\kappa_\mu=\pi\delta_{m1}\frac{k_t}{k}\frac{k_z+sk}{k}\xi\exp\left(-\frac{k_t^2}{2k}\xi\right), \qquad (4)$$

with $\xi\equiv z_R-iz_0$, and

$$z_R=\frac{f^2z_{\rm in}}{z_{\rm in}^2+f^2},\quad z_0=\frac{fz_{\rm in}^2}{z_{\rm in}^2+f^2}. \qquad (5)$$

In general, the expression (3) for the outgoing field must be evaluated numerically. In the paraxial limit ($kz_R\gg1$) z_R and z_0 correspond to the Rayleigh range and the position of the focal plane of the outgoing beam, respectively.

A particular result for the $\vec{\epsilon}_+$ component of $\vec{F}_{\rm out}(\vec{r})$ in the focal region is given in Fig. 1. The focal plane deviates from the paraxial result $z=z_0$ and moves towards the lens by several wavelengths. The size of focal spot for the exact light beam is larger than the corresponding value πw_R^2 with $w_R\equiv\sqrt{z_R\lambda/\pi}$ for a paraxial beam.

With these results in hand, we now investigate the response of an atom located at a position $\vec{r}_0$ in the focal spot (i.e., the position of maximum field intensity) of a strongly focused light beam as in Fig. 1. The goal is to identify the ''maximum'' effect that such an atom can have on the transmitted and scattered fields. We consider a $J_g=0\rightarrow J_e=1$ transition in the atom, as it is the simplest case where all three polarization components of the light in principle play a role. For the cases presented here with the atom located on the z axis, the $\vec{\epsilon}_-$ and $\hat{z}$ components vanish [17], but they can play a dominant role in other situations.

To calculate mean values of the scattered field as well as its intensity and photon statistics, it is convenient to work in the Heisenberg picture. The electric-field operator can be written as the sum of a ''free'' part and a ''source'' part, $\vec{E}=\vec{E}_f+\vec{E}_s$. The source part for the case of a $J_g=0\rightarrow J_e=1$ transition is given by [19]

$$\vec{E}_s^{(+)}(\vec{r})=\sum_i \vec{\Psi}_i(\vec{r}\,')\sigma_i^-(t-|\vec{r}\,'|/c). \qquad (6)$$

We have separated the fields into positive- and negative-frequency components, $\vec{E}_{f,s}=\vec{E}_{f,s}^{(+)}+\vec{E}_{f,s}^{(-)}$, $\vec{r}\,'=\vec{r}-\vec{r}_0$, σ_i^- is the atomic lowering operator, and the sum is over three independent polarization directions $i=\pm1,0$. In the far field, $\vec{\Psi}_i(\vec{r})$ is the dipole field

$$\vec{\Psi}_i(\vec{r})=\frac{\omega_a^2}{4\pi\varepsilon_0c^2}\left[\frac{\vec{d}_i}{r}-\frac{(\vec{d}_i\cdot\vec{r})\vec{r}}{r^3}\right]. \qquad (7)$$

Here $\vec{d}_i=d\hat{u}_i$ is the dipole moment between the ground state $|g\rangle$ and excited state $|e_i\rangle$ in terms of the unit circular vectors $\hat{u}_i$ and the reduced dipole matrix element d.

Expressions containing the electric field in time- and normal-ordered form (as relevant to standard photodetectors) can be calculated using standard quantum-optical methods [19]. E.g., if we assume the initial state of the field incident upon the lens to be a coherent state, the second-order correlation function $G^{(2)}(t,\tau,\vec{r})\equiv\Sigma_{l,m=x,y,z}\langle E_l^{(-)}(t)E_m^{(-)}(t+\tau)E_m^{(+)}(t+\tau)E_l^{(+)}(t)\rangle$ (suppressing the $\vec{r}$ dependence of the fields) consists of 16 terms. For $\tau=0$, seven of these vanish, yielding

$$\begin{aligned}G^{(2)}(t,0,\vec{r})=&|\alpha|^4|\vec{F}_{\rm out}|^4+2\sum_{i,j}|\alpha|^2|\vec{F}_{\rm out}|^2\vec{\Psi}_i^*\cdot\vec{\Psi}_j\sigma_{ee}^{ij}(t_r)\\&+4\sum_i{\rm Re}[\alpha^*\exp(i\omega_at)]\vec{F}_{\rm out}^*\cdot\vec{\Psi}_i|\alpha|^2\\&\times|\vec{F}_{\rm out}|^2\sigma_{eg}^i(t_r)+2\sum_{i,j}|\alpha|^2(\vec{F}_{\rm out}\cdot\vec{\Psi}_i^*)\\&\times[\vec{F}_{\rm out}^*\cdot\vec{\Psi}_j\sigma_{ee}^{ij}(t_r)],\end{aligned} \qquad (8)$$

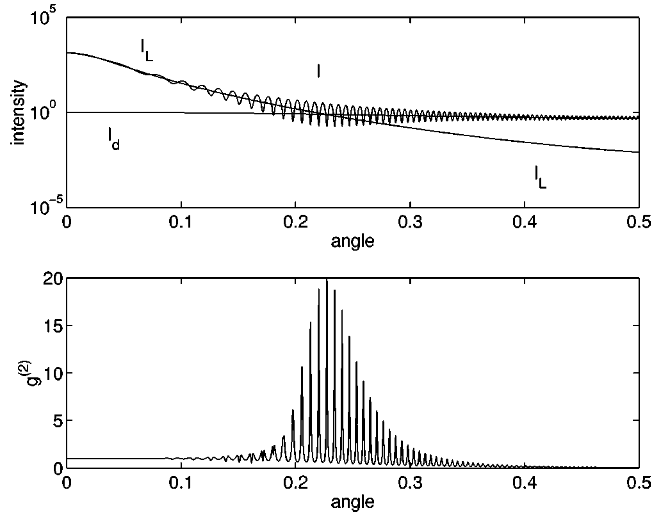

FIG. 2. The intensities $I_L \equiv \langle \vec{E}_f^{(-)} \cdot \vec{E}_f^{(+)} \rangle$ of the laser (free) field $I_d \equiv \langle \vec{E}_s^{(-)} \cdot \vec{E}_s^{(+)} \rangle$ of the dipole (source) field and $I \equiv \langle \vec{E}^{(-)} \cdot \vec{E}^{(+)} \rangle$ of the total field relative to $I_d(\phi=0)$ as a function of the azimuthal angle ϕ/π [i.e., at position $\vec{r}=(R \sin \phi, 0, R \cos \phi)$ where we chose $R=50\lambda$ here and for all further calculations). The parameters for the incoming beam and the lens are as in Fig. 1, and we chose $\lambda = 852$ nm, corresponding to the $D2$ transition in Cs. The atomic dipole moment d is determined by the spontaneous emission rate $\Gamma = 2\pi \times 5$ MHz for the $6P_{3/2}$ states of Cs. (b) $g^{(2)}(0,\vec{r})$ as a function of ϕ/π.

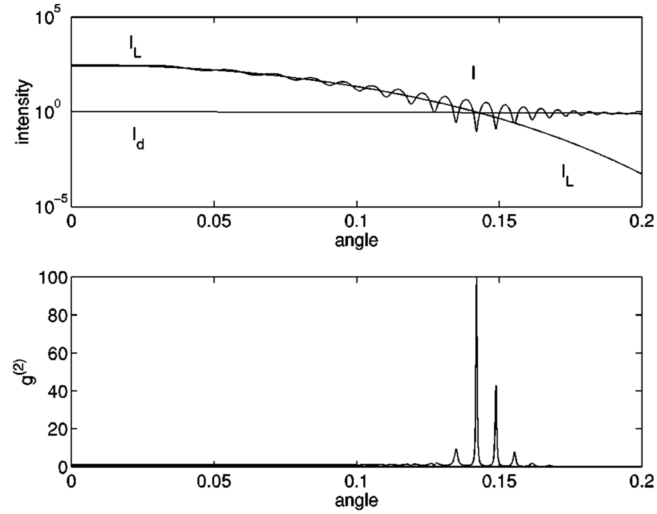

FIG. 3. As Fig. 2, but for a paraxial beam characterized by the same beam parameters $z_R = 4.2\lambda$ and $z_0 = 500\lambda$.

where the coherent-state amplitude is chosen such that $\langle \vec{E}_f^{(+)} \rangle = \alpha \vec{F}_{\text{out}}$, t_r is the retarded time $t_r = t - |\vec{r}\,'|/c$, and $\sigma_{eg}^i = \langle \sigma_i^- \rangle$, and $\sigma_{ee}^{ij} = \langle \sigma_i^+ \sigma_j^- \rangle$ are expectation values of atomic operators. To proceed beyond this point, we must evaluate these atomic quantities. As a simple starting point and in order to make contact with the work of Ref. [9], we assume that the atom reaches a stationary state. Given the value of the electric field at the atom's position $\alpha \vec{F}_{\text{out}}(\vec{r}_0)$, the various atomic expectation values can be straightforwardly derived [19].

For weak ($\alpha \to 0$) on-resonance excitation, we have explicitly evaluated the scattered intensities as well as the normalized second-order correlation function $g^{(2)}(\tau,\vec{r}) \equiv G^{(2)}(\tau,\vec{r})/I^2(\vec{r})$ at $\tau=0$ as functions of position in the far field. Recall that for a stationary steady state, there is no dependence on t. As can be seen in Fig. 2(a), in the forward direction (around $\phi=0$), the free-field contribution $\vec{E}_f$ from the forward propagating incident field overwhelms the source field contribution $\vec{E}_s$ from the atom, even for focusing to a spot of diameter $w_R \approx \lambda$ as in the figure (and in fact is true for any width). This may be compared to a similar result for classical scattering from spherical dielectrics with light focused down to spot sizes larger than five times the size of the spheres [20]. Not surprisingly then, we find that $g^{(2)}(0,\vec{r}) \approx 1$ for forward scattering ($\phi \sim 0$) for *any* input beam, which, however, is in sharp contrast with the result from [9], which would predict a large bunching effect (i.e., $g^{(2)} \gg 1$) for sufficiently tight focusing. If we move instead to large angles ($\phi \sim \pi/2$), Fig. 2(a) shows that the dipole field $\vec{E}_s$ dominates $\vec{E}_f$, so that $g^{(2)}(0,\vec{r})=0$ for $\phi \to \pi/2$ (i.e., the light is almost purely fluorescence and hence antibunched as for plane-wave excitation [21]).

The behavior of $g^{(2)}$ is most interesting around the angle ϕ_0 where the incident $\vec{E}_f$ and source $\vec{E}_s$ fields have the same magnitude. Indeed, the oscillations apparent in Fig. 2(b) indicate that $g^{(2)}(0,\vec{r})$ is very sensitive to the relative phase between $\vec{E}_f$ and $\vec{E}_s$. Maxima in $g^{(2)}$ appear when the free field and the dipole field interfere destructively. Adapting the interpretation of Carmichael and Kochan [9] from an essentially one-dimensional setting to the angular dependence of the fields around ϕ_0, we see that this implies that a photon has just been absorbed by the atom, which is therefore in its excited state, so that a fluorescent photon can be expected to appear soon, thus leading to strong bunching. We suggest that the combined angular dependences of $I(\vec{r})$ and $g^{(2)}(0,\vec{r})$ evidenced in Figs. 2 and 3 are characteristic of scattering from a *quantum aperture* such as an atom in free space.

We have compared these exact 3D results with those for a Gaussian beam with the same parameters z_0 and z_R. In qualitative terms, a Gaussian beam exaggerates the amount of light in the forward direction at the cost of greatly underestimating it for larger angles. This implies that the region where $g^{(2)}$ reaches its maximum is moved to smaller angles ϕ for a paraxial beam (for the parameters of Fig. 2, $\phi_0 \sim 26°$ compared to $\phi_0 \sim 40°$, respectively). Moreover, the value of that maximum is exaggerated as well, with a maximum value of $g^{(2)}(0,\vec{r}) \sim 100$ for the Gaussian beam. For even stronger focusing, there will be large bunching at $\phi = 0$ for a paraxial beam, as in [9], but, as mentioned before, not for the exact solutions.

Finally, we come back to the issue raised at the beginning of this paper: Why does focusing a light beam to size σ not give rise to large effects? One simple answer is that there is a limit to how strongly one can focus a light beam [22], as indeed our exact solutions show with focal areas A always larger than σ. Moreover, for tightly focused beams, the polarization state in the focal volume is anything but spatially uniform, so that the field associated with a single polarization for a paraxial input is split among various components. In fact, if the atomic dipole is $\vec{d}=d\hat{u}$, the relevant quantity determining the excitation probability is $|\hat{u}\cdot\vec{E}^{(-)}(\vec{r}_0)|^2$ evaluated at the atom's position $\vec{r}_0$, while the total intensity in the focal plane is given by $\int dS|\vec{E}^{(-)}|^2$. Thus, instead of $R=\sigma/A$, the scattering ratio R_s is

$$R_s=\frac{3\lambda^2|\hat{u}\cdot\vec{E}^{(-)}(\vec{r}_0)|^2}{2\pi\int dS|\vec{E}^{(-)}|^2}. \tag{9}$$

For a paraxial beam $R_s=2\sigma/(\pi w_R^2)\ll 1$. For the lens parameter used here, $f=500\lambda$, the optimum value (i.e., optimized over the parameters of the incoming beam) for R_s is 10%. Note that the ratio of the intensities of scattered ($\vec{E}_s$) and laser fields ($\vec{E}_f$) in the forward direction ($\phi=0$ in Fig. 2) is much smaller than that (about 10^{-3}), because the laser beam channels much more power in that direction than does the dipole field.

For extreme values of f on the order of λ, the maximum scattering ratio does increase, but not beyond 50%. Even for a scattering ratio of close to 50% (reached for $f=2\lambda$ and $z_{\mathrm{in}}=4\lambda$, for instance), the ratio of laser field intensity I_L to scattered intensity I_d in the forward direction ($\phi=0$) is not small, namely about 21. Moreover, the value for $g^{(2)}(\tau=0)=0.95$ agrees with Ref. [9] in the sense that for the parameter $\Gamma\approx 0.5$ from that paper antibunching is indeed predicted. On the other hand, it is in contrast with the suggestion made there that very strong bunching results for focusing to an area $A\sim\sigma$. Finally, note that the upper limit of 50% for R_s can be understood by noting that the optimum shape of the illuminating field would be a dipole field. Here with light coming only from one direction, one may indeed expect R_s to be at most 1/2. With one mirror behind the atom, an improvement in the scattering ratio by about a factor of 2 might be expected. And of course, by building an optical cavity around the atom, the atom-light interaction can be further enhanced by orders of magnitude as in cavity quantum electrodynamics [23].

In conclusion, by strongly focusing light on a single atom in free space, one may create an appreciable light-atom interaction, which, however, is not as strong as might be naively expected. On the one hand, this implies that a coherent-state field employed for ''classical'' addressing of a single atom in implementations of quantum computing and communication [4,6,7] carries little information about that atom, so that entanglement of the atom with other atoms in a quantum register can be preserved. On the other hand, there are serious obstacles associated with using a single atom to process quantum information encoded in single photons in free space.

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