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Calculations of the Atom-wave Modal of a Restricted Atom in a Two-dimensional Potential

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Abstract. We investigate the atom-wave modal of the neutral atom restricted by the two-dimensional optical dipole potential due to a cavity mode. Our model is based on the optical restriction of a sodium atom inside a long hollow cylinder with a rectangular cross section of sub-wavelength dimensions $a \times b$. We have assumed large negative detuning situation $\delta \gg \Re_0, \gamma_0$ and that the atom dipole moment vector d is set in the longitudinal direction. The parameters selected in this work are taken to guarantee that the atom is sufficiently cooled below the recoil limit to permit several quasi harmonics restricted quantum states.

Introduction

The study of the motion of atoms in laser light fields has led to remarkable advance in atom cooling and restricting (trapping) [1-5]. In particular, the intense coherent light of laser has been used to cool neutral atoms down to the micro-Kelvin [6] and now even the nano—Kelvin regimes [7]. At such low temperatures, the de Broglie wavelike character of the atom becomes pronounced, making it necessary to treat the atom as wave phenomena.

The atom-wave modal of such atom is fully achieved by solving Schrödinger equation to find the vibrational wave functions and evaluating the discrete vibrational quantum states [8]. Recently, the Schrödinger modal of restricted atom has received considerable attention. Starting with the work of Wallis *et al*. in 1992, three different cases of opening cavities; parabolic atomic mirror, evanescent light-wave and gravitational trap have been calculated [9]. Dowling in 1993, Dowling and Gea-Banacloche in 1994 and 1995 and Söding *et al.* in 1995 have carried out the same calculation for conical and pyramidal traps [10-12]. We have evaluated such modal for an atom restricted between parallel-plate by the optical dipole potential [13].

The main objective of this paper is to consider the problem of finding the atom-wave modal for a restricted atom inside a long hollow cylinder with a rectangular cross section of sub-wavelength dimensions by solving Schrödinger equation. In contrast to opening and parallel-plate cavities, the rectangular waveguide gives sufficient depth to the potential well at the same set of parameters. In addition, the rectangular waveguide can also confine atoms transversely in two directions which leads the elimination of the problems of the transverse diffusion that limit the ability of the parallel plates waveguide [14-15].

The paper is organized as follows. In Section 2, we present the theoretical model of this study that deals with an optically restricted single atom inside a long hollow cylinder with a rectangular cross section. In addition, we outline the procedure leading to the evaluation of the two-dimensional optical restricting potential in such a cavity. In Section 3, we estimate the vibrational frequency of the restricted atom by using the harmonic oscillator approximation. In Section 4, we derive the numerical solution of the two-dimensional Schrödinger equation involving the full potential leading to the precise details of the vibrational levels using sodium atom for illustration. Section 5 contains the conclusions.

2. Theoretical Model

The atom guide focused on here is in the form of a rectangular waveguide, as depicted in Fig. 1. As shown in this figure, a normal cross section is assumed to have the dimension $a \times b$ and is taken to lie in $y-z$ plane with the cylinder axis along the x direction, coinciding with the straight line $y = b/2$; $z = a/2$. The guide is bounded by walls arising from the intersection of four planes at $y = 0$; $y = b$ and $z = 0$; $z = a$, all are assumed to be planar surfaces of perfect conductors which exclude all electromagnetic fields from their interior. The standard electromagnetic boundary conditions apply such that the tangential component of the electric field vector and magnetic field vector must vanish at every point on all guide walls.

The optical dipole potential of such model can be altered fundamentally when a waveguide mode is excited at frequency $\omega(k_{\|}, n, m)$, which is nearly tuned to the dipole transition frequency ω_0. The mode frequency satisfying the dispersion relation:

$$\omega\left(k_{\|}, m, n\right) = c\left(k_{\|}^{2} + \frac{m^2\pi^2}{b^2} + \frac{n^2\pi^2}{a^2}\right)^{1/2} \tag{1}$$

where m and n are the integer quantum numbers refer to the order of excited mode and $k_{\|}$ is an axial wave vector.

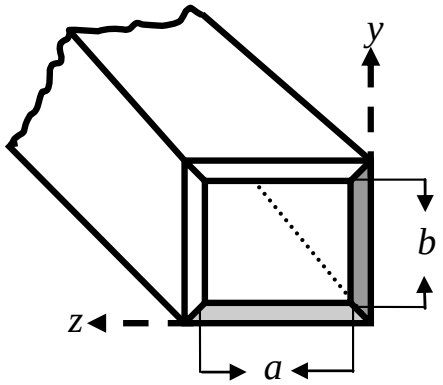

Fig. 1. A rectangular waveguide.

It is convenient to simplify the notion by introducing a compound mode variable q which stands for the three-mode variable $(k_{\|}, m, n)$. By setting $\mathbf{r} = (x, \mathbf{r}_{\perp})$ with x an axial coordinate and $\mathbf{r}_{\perp} = (y, z)$ at a two-dimensional (transverse) position vector in the $y-z$ plane, we can write the optical dipole potential U that confines the atom inside a rectangular waveguide at a static case as [5]:

$$U\left(q, \mathbf{r}_{\perp}\right) = \left\{ \left(\frac{\hbar \delta(q, \mathbf{r}_{\perp})}{2} \right) \ln \left[1 + \frac{2\Re^2(q, \mathbf{r}_{\perp})}{\left[\delta^2(q, \mathbf{r}_{\perp}) + \gamma^2(\mathbf{r}_{\perp}) \right]} \right] \right\} \tag{2}$$

where $\gamma(\mathbf{r}_{\perp})$ is the spontaneous emission rate, $\Re(k_{\|}, m, n, \mathbf{r}_{\perp})$ is Rabi frequency and $\delta = \omega(q) - \omega_0$ is the static detuning of the cavity mode from the atomic resonance. Here, we are going to consider just an especial situation for the spontaneous emission rate $\gamma(\mathbf{r}_{\perp})$, Rabi frequency $\Re(q, \mathbf{r}_{\perp})$ and thus the optical dipole potential $U\left(q, \mathbf{r}_{\perp}\right)$. In that the atom is orientated parallel to the axial direction of the waveguide with negative detuning $\delta < 0$. In addition, the parameters selected in our evaluation are taken to guarantee that the atom is sufficiently cooled below the recoil limit. We have applied these conditions because the main aim of this work is to evaluate a quantum behavior of the neutral atom restricted by two-dimensional guiding potential. In this situation, Eq. (2) should be re-written as follows:

$$\mathrm{U}_{\|}\left(\mathrm{q}, \mathbf{r}_{\perp}\right) = \left\{ \left(\frac{\hbar \delta(\mathrm{q}, \mathbf{r}_{\perp})}{2} \right) \ln \left[1 + \frac{2\Re_{\|}^2(\mathrm{q}, \mathbf{r}_{\perp})}{\left[\delta^2(\mathrm{q}, \mathbf{r}_{\perp}) + \gamma_{\|}^2(\mathbf{r}_{\perp}) \right]} \right] \right\} \tag{3}$$

To ease the calculation, we suppose that $a = b = L$, therefore the spontaneous emission rate $\gamma_{||}(\mathbf{r}_{\perp})$ can be given by [15]:

$$\gamma_{||}(\mathbf{r}_{\perp}) = \gamma_o \sum_{m=0}^{[2L/\lambda]} \sum_{n=0}^{[2L/z]} \frac{3\lambda^3}{4\pi L^2} \left[\frac{m^2 + n^2}{\left(\frac{\omega_0^2 L^2}{\pi^2 c^2} - m^2 - n^2 \right)^{1/2}} \right] \sin^2\left(\frac{m\pi y}{L} \right) \sin^2\left(\frac{n\pi z}{L} \right) \qquad (4)$$

where γ_0 is the corresponding spontaneous rate in free space. Beside $m = 1$ and $n = 1$ for the p-polarized case, $\Re_{||}(k_{||}, 1, 1, \mathbf{r}_{\perp})$ can be given by [15]:

$$\Re_{||}(k_{||}, 1, 1, \mathbf{r}_{\perp}) = \Re_0 \left(\frac{2\pi c}{\omega_0 L} \right) \sin\left(\frac{\pi y}{L} \right) \sin\left(\frac{\pi z}{L} \right) \qquad (5)$$

where $\Re_0$ is the corresponding Rabi frequency in free space.

Figure 2 shows the variation of the optical dipole potential $U(k_{||}, 1, 1, \mathbf{r}_{\perp})$ for sodium atom when its dipole orientated parallel to the axial direction of the waveguide corresponding to the parameters given in Table 1.

Table 1. The parameters corresponding to Figs. 2, 3 and 4

Parameters	Symbol	Value	Units
Free space wavelength	λ	589	*nm*
Atomic mass	M	3.8×10^{-26}	*kg*
Waveguide length	L	$1.5\,\lambda / 2$	*nm*
Free space decay rate	γ_0	61.3	*MHz*
Free space Rabi freq.	$\Re_0$	8.56	*GHz*
Static detuning	δ	- 36.78	*GHz*

It can be seen from Fig. 2 that, the central well depth is about $23.5u$ (where $u = 2.6 \times 10^{-26}$ J) which is very enough deep to permit several quasi harmonic vibrational quantum states. The vibrational frequency of the quantum states can be estimated simply by using the harmonic oscillator approximation while the precise details of these states can be obtained straightforwardly by the numerical solution of the two-dimensional Schrödinger equation involving the full potential.

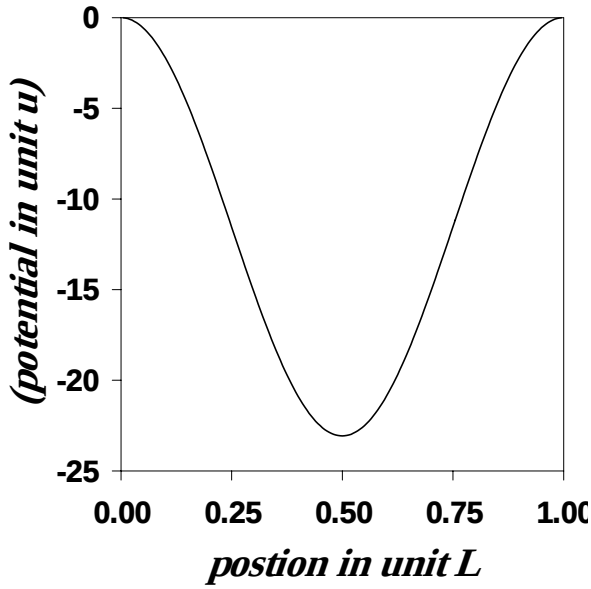

Fig. 2. Cross section of the optical dipole potential of the atom inside the rectangular waveguide.

3. Harmonic Oscillator Approximation

We can estimate the vibrational frequency of the restriction of such atom by approximating the dipole potential in Fig. 2 by the harmonic oscillator approximation around the dipole potential minimum for mode m, n as [16]:

$$U(q, \mathbf{r}_{\perp}) \approx U_{\min.} + \frac{1}{2} M\omega_{mn}{}^{2} (\mathbf{r} - \mathbf{r}_{\min})^{2} + ... \tag{6}$$

where ω_{mn} is the vibrational frequency of the atom in the dipole potential and the sub-numbers refer to the order of the excited mode. The quantity $M\omega_{mn}$ is called the Stifness constant and $U_{\min.}$ is the potential minimum which can be given by:

$$U_{\min}(k_{\|}, m, n, \mathbf{r}_{\perp}) = \left\{ \left(\frac{\hbar\delta}{2} \right) \ln \left[1 + \frac{2\Re_{\|}^{2} (k_{\|}, m, n, \mathbf{r}_{\min})}{\left[\delta^{2} + \gamma_{\|}^{2} (\mathbf{r}_{\min}) \right]} \right] \right\} \tag{7}$$

The harmonic oscillator approximation for the parameters given in Table 1 is going to give a central well depth approximately like Fig. 2 as shown clearly by a dotted line in Fig. 3.

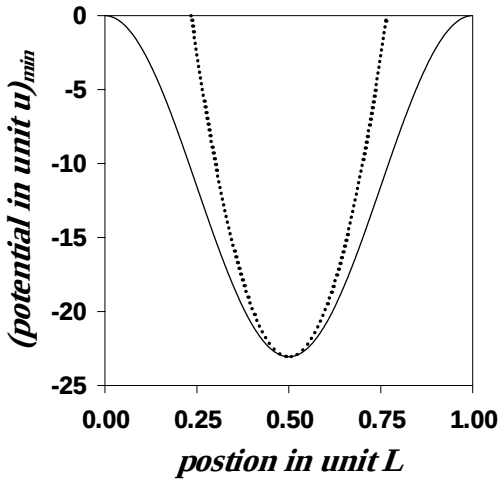

Fig. 3. The cross section of the optical dipole potential of the atom inside the rectangular waveguide showing the potential minimum at the center. The dotted line shows the harmonic oscillator approximation to the dipole potential.

The harmonic vibrational frequency ω_{mn} can be estimated simply by using the harmonic oscillator approximation as follows:

$$\omega_{\mathrm{mn}} = \left\{ \frac{2}{\mathrm{M}} \nabla_{\perp}^{2} \mathrm{U}(\mathrm{q}, \mathbf{r}_{\perp}) \right\}_{\mathbf{r}_{\mathrm{min}}}^{\frac{1}{2}} \tag{8}$$

where $\nabla_{\perp}^{2} = \partial^2 / \partial \mathrm{y}^2 + \partial^2 / \partial \mathrm{z}^2$ is the Laplacian operator for the cross-sectional coordinate. We have explicitly,

$$\omega_{\mathrm{mn}} = \left\{ \frac{4\hbar\pi^2 \Re_{\parallel}^{2}(\mathrm{q}, \mathbf{r}_{\perp})\delta}{\left[\delta^2 + 2\Re_{\parallel}^{2}(\mathrm{q}, \mathbf{r}_{\perp}) \right] \mathrm{L}^2 \mathrm{M}} \right\}_{\mathbf{r}_{\mathrm{min}}}^{\frac{1}{2}} \tag{9}$$

while the corresponding harmonic oscillator approximation ground state width of the atom is obtained by:

$$\Delta \mathbf{r} = \left(\hbar / \mathrm{M}\omega_{\mathrm{mn}} \right)^{1/2} \tag{10}$$

The harmonic oscillator approximation is valid only if $\Delta \mathbf{r} << \mathbf{r}$ so that the atomic wave function is well localized around the potential minimum. It is not difficult to check that for the above parameters values for sodium atom immersed in $m = n = 1$ p-polarized mode within the rectangular waveguide system described above we have:

$$\omega_{11} \approx 19.1\mathrm{MHz} \tag{11}$$

4. The Schrodinger Equation

The calculation of the atom-wave modal can be obtained by solving a scalar wave equation in a rectangular waveguide. In this case, the Schrödinger equation of such system may be written as:

$$-\frac{\hbar^2}{2\mathrm{M}}\left(\nabla_{\perp}^2 - \mathrm{k}_{\parallel}^2 \right) \Psi_{\mathrm{q}}(\mathbf{r}) + \left[\mathrm{U}\left(\mathrm{k}_{\parallel}, 1, 1, \mathbf{r}_{\perp} \right) - \mathrm{E} \right] \Psi_{\mathrm{q}}(\mathbf{r}) = 0 \tag{12}$$

where $\mathrm{U}\left(\mathrm{k}_{\parallel}, 1, 1, \mathbf{r}_{\perp} \right) \equiv \mathrm{U}_{11}(\mathrm{k}_{\parallel}, \mathbf{r}_{\perp})$ is the optical dipole potential that the atom is immersed in, which varies with waveguide cross-section according to Fig. 2 and E is the vibrational energy eigen-value. $\Psi_{\mathrm{q}}(\mathbf{r}_{\perp})$ is the wave-function of the moving atom inside the rectangular waveguide and for the parallel case of p-polarized mode, which can be easily given by:

$$\Psi_{\mathrm{q}}(\mathbf{r}) = \mathcal{N}_{\mathrm{p}}(\mathrm{q}) \left(\mathrm{m}^2 + \mathrm{n}^2 \right) \pi^2 \mathrm{L}^{-2} \sin\left(\frac{\mathrm{m}\pi \mathrm{y}}{\mathrm{L}} \right) \sin\left(\frac{\mathrm{n}\pi \mathrm{z}}{\mathrm{L}} \right) \exp \mathrm{i}(\mathrm{k}_{\parallel} \mathrm{x}) \tag{13}$$

where $\mathcal{N}_{\mathrm{p}}(\mathrm{q})$ is the p-polarized mode normalization factor given by:

$$\mathcal{N}_p^2(\mathrm{q}) = \left(\frac{2\hbar \mathrm{c}^2}{\mathrm{L}\varepsilon_0 \pi^2 \omega(\mathrm{q}) \left(\mathrm{m}^2 + \mathrm{n}^2 \right)} \right) \tag{14}$$

By rearranging the Eq. (12), we have:

$$\left[\nabla_{\perp}^2 - \mathrm{k}_{\parallel}^2 \right] \Psi_{\mathrm{q}}(\mathbf{r}) + \frac{2\mathrm{M}}{\hbar^2} \left[(\mathrm{E} - \mathrm{U}_{11}(\mathrm{k}_{\parallel}, \mathbf{r}_{\perp}) \right] \Psi_{\mathrm{q}}(\mathbf{r}_{\perp}) = 0 \tag{15}$$

Performing the change of variables $\mathcal{S} = y / L$ and $\mathcal{S}' = z / L$, yields:

$$\left[\frac{\mathrm{d}^2}{\mathrm{d}\mathcal{S}^2}+\frac{\mathrm{d}^2}{\mathrm{d}\mathcal{S}'^2}-\mathrm{k}_{\|}^2\mathrm{L}^2\right]\Psi_{\mathrm{q}}(\mathcal{S},\mathcal{S}')+\frac{2\mathrm{ML}^2}{\hbar^2}\left[(\mathrm{E}-\mathrm{U}_{11}(\mathrm{k}_{\|},\mathcal{S},\mathcal{S}')\right]\Psi_{\mathrm{q}}(\mathcal{S},\mathcal{S}')=0 \tag{16}$$

The energy E and the potential U can be scaled to the dimensionless quantities $\Xi=\mathrm{E}/\mathrm{E}_0$ and $\mathrm{V}=\mathrm{U}/\mathrm{E}_0$ by introducing the quantity $\mathrm{E}_0=\hbar^2/2\mathrm{ML}^2$. Then Eq. (16) becomes:

$$\left[\frac{\mathrm{d}^2}{\mathrm{d}\mathcal{S}^2}+\frac{\mathrm{d}^2}{\mathrm{d}\mathcal{S}'^2}\right]\Psi_{\mathrm{q}}(\mathcal{S},\mathcal{S}')+\left[\Xi-\mathrm{V}_{11}(\mathrm{k}_{\|},\mathcal{S},\mathcal{S}')-\mathrm{k}_{\|}^2\mathrm{L}^2\right]\Psi_{\mathrm{q}}(\mathcal{S},\mathcal{S}')=0 \tag{17}$$

Let us assume that the atom is subjected to a sufficient cooling process before it is coupled to the waveguide (i.e. $\vartheta\approx 0$). This leads to that the value of the longitudinal wave-vector $k_{\|}$ considered quantized and consequently, the system operate with particular longitudinal mode of propagation (i.e. single mode operation). In this case, the maximum transverse velocity $\vartheta_{\perp}$ due to the potential, which corresponds to the central potential depth, can be given as [13]:

$$\vartheta_{\perp(\max)}=\left[2\mathrm{U}_{11}(\mathbf{r}_{\perp}=\mathrm{L}/2)_{\min}/\mathrm{M}\right]^{1/2} \tag{18}$$

Here, the maximum transverse velocity $\vartheta_{\perp(\max)}$ is $5.56\,m/s$, therefore the momentum of the photon is analogous to the momentum of the atom or, in other words, the de Broglie atomic wavelength is large enough to observe. Consequently, from the boundary condition $\Psi_{\mathrm{q}}(\mathrm{y},\mathrm{z}=0)=\Psi_{\mathrm{q}}(\mathrm{y},\mathrm{z}=\mathrm{L})=0$ at the hollow wall and the localization of the atom at the centre of the waveguide $\mathrm{V}_{\mathrm{mn}}(\mathcal{S},\mathcal{S}'=1/2)\equiv\mathrm{V}_{\mathrm{mn}}$, the transverse quantization condition is:

$$\Xi_{\mathrm{mn}}=\mathrm{V}_{\mathrm{mn}}+\mathrm{k}_{\mathrm{mn}}^2\mathrm{L}^2+\pi^2(\mathrm{m}^2+\mathrm{n}^2) \tag{19}$$

However, the eigen-value Eq. (17) can be solved numerically with high accuracy in many ways [17]. It can be deduced from Eq. (13) that the lowest wave-function will be Ψ_{11} because Ψ_{00}, Ψ_{01} and Ψ_{10} will be zero. We plot the atom wave-functions Ψ_{mn} where $n,m=1,2,3$ in Fig. 4 at $x=0$. These are exactly the same as the normal solution to the two-dimensional harmonic oscillator problem. It can be seen that, in the rectangular waveguide when $a=b\equiv L$ (i.e. the square waveguide case), Ψ_{12} has exactly the same shape and magnitude as Ψ_{21} with different orientation because these two modes have the same dispersion relation. This property will be true for any two-commutative modes in the square waveguide. In contrast to the case $a\neq b$, one of the

commutative modes will have the lesser value of dispersion relation depending on the shorter direction. This also leads to the same shape of wave-function, but with a different magnitude.

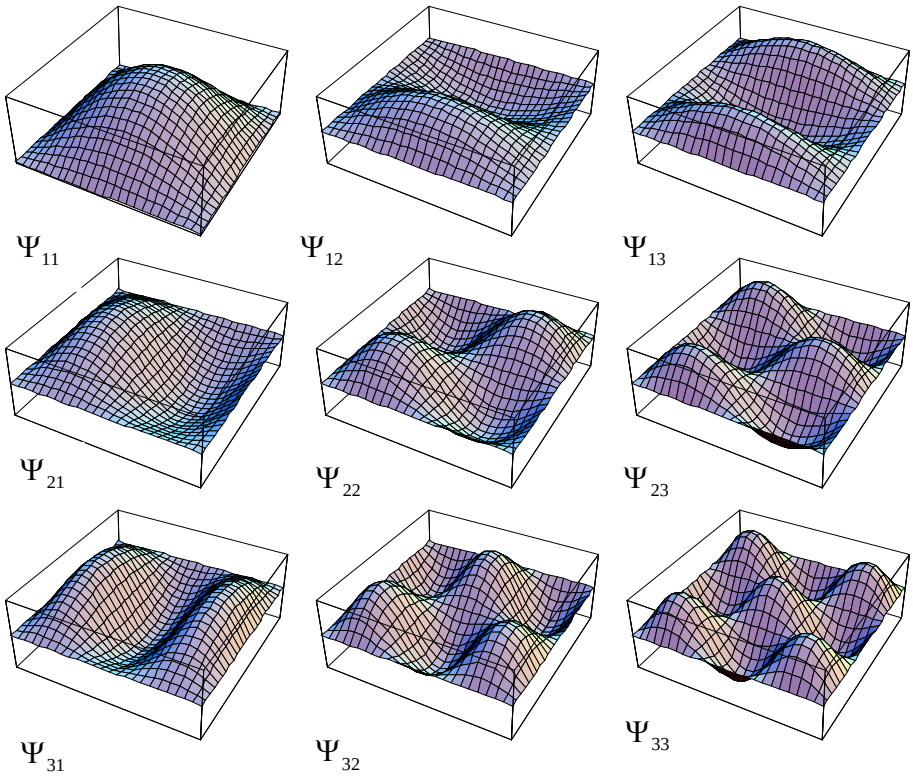

Fig. 4. First six-wave function for a single mode atom wave propagation in red-detuned inside the rectangular waveguide.

The relationship between the transverse temperature, waveguide dimension and mode propagation can be defined in a transverse de Broglie wavelength $\lambda_{mn}^{\perp}$ as follows:

$$\lambda_{mn}^{\perp} = \frac{2L}{(m^2 + n^2)^{1/2}} \tag{20}$$

while the transverse attenuation constant α_{mn} through the waveguide cross section can be obtained in the view of Eq. (19) as:

$$\alpha_{mn} = \left(\Xi_{mn} - V_{mn} - k_{mn}^2 L^2\right)/L \tag{21}$$

For good, single mode, coherent atomic beam, one would like to use the lowest order Ψ_{11} mode. This mode requires the lowest transverse temperature and the largest transverse de Broglie wavelength, $\lambda_{11}^{\perp} = 2L$. This result is commonly accepted with the basic idea of the wave optics approach, where one assumes that the wave is confined within the hollow of the waveguide with a standing wave pattern in the lateral direction that falls to zero at the hollow wells and an integral number of half-wavelengths are fitted across the cross section of the waveguide.

The transverse temperature $T_{mn}^{\perp}$ (in degree Kelvin) required to attain these transverse de Broglie wavelengths are given by:

$$T_{mn}^{\perp} = \frac{\hbar^2\pi^2\left(m^2 + n^2\right)}{2Mk_B L^2} \tag{21}$$

For the lowest order Ψ mode corresponding to the parameters given in Table 1, Eq. (21) yields transverse temperature of $T_{11}^{\perp} \approx 0.53\mu K$ which is only less by 4.52 times then the recoil temperature for sodium atom $(T = 2.4\,\mu K)$. However, the cooling of atoms to below recoil temperature by as much as $(T/70)$ has been achieved experimentally [7].

5. Conclusions

In conclusion, we have examined in detail the quantum properties of restricted atoms in waveguide with the hollow rectangular cross section. The optical potential that acts on the atom with negative detuning to restrict the atoms within the central region was evaluated. This evaluation was made using appropriate parameters that provide a adequately deep central well.

We have also calculated transverse atomic motion of the atom in the restricting potential due to a system mode and described this motion in terms of quantum states in two ways. First, we have estimated the vibrational frequency of these quantum states using the harmonic oscillator approximation. Second, we have evaluated them by the numerical solution of the two-dimensional Schrödinger equation.

It should be noted that here we have neglected the effect of the gravity, but it has been considered by Harris and Savage [18]. In addition, the problems of the van deer Waals potential which effectively acts at short distances $(L << \lambda/4\pi)$ and the Casimir-

Polder at large distances $(L >> \lambda / 4\pi)$ is also not considered, but they have been clearly estimated by Sukenik *et al.* [19] as well as by Marksteiner *et al.* [20].

Finally, the researcher would like to mention that the major benefit of such work arises from the fact that it provides a more extensive understanding of the quantum behavior of a restricting atom in a micro-cavity, in general. Along with, there are some arguments that such a confinement is useful in the study of Bose-Einstein condensation and basically can be used in quantum information processing [21-23].

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حساب النمط "الموجي-الذري" لذرة مأسورة في جهد ثنائي البعد

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(قدم للنشر في ١٤٢٦/٢/١١هـ؛ وقبل للنشر في ١٤٢٨/٣/٢٨هـ)

ملخص البحث. لقد ركز البحث على حساب النمط "الموجي-الذري" وذلك لذرة متعادلة مأسورة بواسطة جهد بصري ثنائي البُعد ناتج عن إثارة نمط فجوة، ويعتمد النظام الفيزيائي المستخدم كليًّا على الأسر البصري لذرة صوديوم تتحرك على طول تجويف أسطواني ذو مقطع عرضي مستطيل الشكل له أبعاد $a\times b$ في مدى أقل من الطول الموجي المستعمل، وأما بالنسبة لتوليف نمط الفجوة البصرية المثار فقد تم استخدام توليف عالي سالب بحيث يمكن التأكيد أن معدل الانبعاث التلقائي للذرة γ_0 ، وكذلك تردد رابي لها $\Re_0$ ، لهما قيمة أقل بكثير من قيمة هذا التوليف (أي أن: $\delta \gg \Re_0, \gamma_0$)، وفي الوقت نفسه فقد تم افتراض أن عزم ثنائي القطب للذرة $\mathbf{d}$ سيكون متجهًا فقط صوب الإحداثي الطولي للفجوة البصرية، وأما بالنسبة لبقية المتغيرات الديناميكية فقد جرى اختيارها بحيث يتم توفير تبريد كافي للذرة تحت حد ارتدادها الطبيعي؛ وذلك من أجل ضمان الحصول على مستويات أسر كمية شبه توافقية.