Strongly coupled cold atoms in bilayer dense lattices

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Abstract
We theoretically investigate the optical response of many cold atoms within a pair of identical planar lattices mostly in a dense regime using microscopic electrodynamics numerical simulations. We find cooperative optical properties of the double atomic lattices to a normal incidence of low-intensity radiation at particular ranges of sample parameters. The main findings are that resonance shifts, linewidths, and transmittance could be engineered by varying layer-to-layer distance, lattice constant, and parameters for incident light. We also propose a bilayer atomic lattice could be modeled as two effective superatoms. Simulation results qualitatively agree with the ones from an isotropic infinite lattice model in the ranges of external parameters for which a mean-field approximation is not valid. Hopefully, our bilayer lattice samples might be exploited for implementing an optical switch and a photonic device in quantum computing.

1. Introduction
Owing to advances in trapping techniques [1] for laser or evaporatively cooled atoms, a sample of effectively stationary atoms is experimentally manipulated and engineered to explore light–matter interaction at the most fundamental level. Moreover, there is a growing interest in light propagation through a nanometer-size sample of homogeneously broadened (i.e. low-temperature) atoms with a sufficiently high number density due to potential applications in the areas of efficient light transport [2], quantum information processing [3], metamaterials [4], integrated optical devices [3], and nano-optics [6]. Recently realized experiments [7–11] for cold dense atoms motivate theoretical investigations [12–24] of light propagation at the microscopic level. Even if responses of a single two-level atom to the incident radiation have been fairly well known, optical behaviors of an aggregation of two-level atoms are far more elusive. In particular, for a homogeneously broadened sample in close proximity, atoms move distances on the order of the resonant wavelength over the time for internal state to relax to steady-state. The total field on each atom is then expressed by the field scattered from the other atoms as well as the incident field. Consequently, sample atoms are strongly correlated and their behaviors can be explained by solving highly coupled dynamics that is self-consistently described.

Prior studies developed theoretical formalisms for a two-dimensional (2D) cold atom lattice driven by external radiation [16]. In this study, we extend the formalism to a pair of coupled 2D lattices in the high density regime. Light pressure and effects of photon recoils of the steady-state atoms are all neglected. Furthermore, low light intensity is considered so that the atomic lattices driven by the external light are well approximated as dipoles with fixed positions and described by the coupled-dipole equations [12–17, 22]. We obtain local fields seen by dipoles at their positions by solving the coupled-dipole equations. For a two-atom sample we present analytical solutions for transmittance and optical thickness. Exact solutions for many-atom lattices are obtained numerically for cooperative resonance shifts, linewidths, and optical spectra. Our main finding is that cooperative optical responses of bilayer samples such as splitting of the absorption lines, which are observed at a high atomic density of the monolayer plane [16] or a small plane-to-plane distance, cannot be explained by the standard optics theory based on an electrodynamics of a polarizable medium (EDPM) [25]. In fact, the EDPM is the effective-medium mean-field theory (MFT) which approximates the local fields of atoms to be the same
everywhere, so it cannot properly describe the physics of a sample with a nanometric size. Therefore, we need to resort to large-scale simulations as a way to understand the optical behaviors of cold dense many-atom samples.

In the regime of high atomic density and small interlayer separation, we validate our theoretical approaches and numerical simulations by comparing line shifts with analytical results for a two-atom sample and for an isotropic and infinite lattice model. In the low atomic density regime, standard optics theory confirms the validity of simulation results. It is predicted that under certain conditions, the transmittance of cold dense atoms can realize on- and off-states and therefore is a candidate system for a photonic device in quantum computing [13, 17]. Finally, we discuss that each monolayer of a bilayer lattice could be modeled as an effective superatom acting as a mirror [26] with amplitude reflection and transmission coefficients [27] which makes it convenient for applying a Fabry–Pérot interferometer.

2. Microscopic electrodynamics simulation

Our approach is based on earlier quantum-field theory [28] of light propagation through dipolar medium where field operators describe ground-state and excited-state atoms coupled to the quantized electromagnetic field via the dipole interaction. In the limit of low light intensity for a particular atomic transition from the ground-level to a position \( \mathbf{r}_i \) reads

\[
\mathbf{P}(\mathbf{r}_i) = (i\Delta - \gamma)\mathbf{P}(\mathbf{r}_i) + i\zeta\mathbf{E}_0(\mathbf{r}_i)\rho(\mathbf{r}_i) + i\zeta\rho(\mathbf{r}_i)\int d^3r_2\mathbf{G}(\mathbf{r}_i, \mathbf{r}_2)\mathbf{P}(\mathbf{r}_2).
\]  

(1)

Here \( \Delta = \omega - \omega_0 \) is the detuning of the incident light with angular frequency \( \omega \) with respect to the atomic transition frequency \( \omega_0 \), \( \gamma \) is the HWHM linewidth of the optical transition, \( \mathbf{E}_0 \) the electric field in the absence of matter, and \( \rho \) the atomic density. \( \mathbf{G}(\mathbf{r}_i, \mathbf{r}_2) \) represents the monochromatic dipole field propagator [16] such that \( \mathbf{G}(\mathbf{r}_i, \mathbf{r}_2) \) expresses the electric field at \( \mathbf{r}_2 \) due to an oscillating dipole moment \( \mathbf{d} \) at \( \mathbf{r}_i \). We also define \( \zeta = \frac{D^2}{\hbar} \) in which the reduced dipole matrix element \( D \) is related to the transition linewidth \( \gamma \) and the wavenumber \( k_0 = 2\pi/\lambda_0 = \omega_0/c \) of resonant light with wavelength \( \lambda_0 \) by

\[
\gamma = \frac{D^2k_0^3}{6\pi\hbar c}.
\]

(2)

With the solution of equation (1) given, the expectation value of the electric field is expressed as

\[
\mathbf{E}(\mathbf{r}) = \mathbf{E}_0(\mathbf{r}) + \int d^3r'\mathbf{G}(\mathbf{r}, \mathbf{r}')\mathbf{P}(\mathbf{r}').
\]

(3)

In the present theoretical scheme we do not include the motion of the atoms, light pressure, and effects of photon recoil. Equation (1) is obtained under assumption that there are no correlations between the positions and dipole moments of the atoms so that it is a mean-field equation for atomic density and polarization. In such a mean-field approximation polarization is treated as a continuous field. As a result, the information about the precise atomic positions and light-mediated correlations are all lost.

A prescription from a microscopic electrodynamics now enters into the theoretical scheme in order to fix its mean-field nature: we assign the positions of all two-level atoms in a pair of identical and parallel 2D square lattices with \( N \) sites each filled with one point-like cold atom. Positions of the atoms \( \mathbf{R}_i(i = 1, 2, \ldots, 2N) \) within the sample are generated deterministically such that light-mediated correlations are not initially built in the sample. Therefore, our simulation with fixed atomic positions differs from stochastic coupled-dipole numerical simulations [14, 15, 18, 22, 29] with random atomic positions. We assume that atoms in the lattice sites are in a steady-state and do not tunnel into the other sites, leading to the dipole moments of the atoms

\[
d(\mathbf{R}_i) = \alpha\left[\mathbf{E}_0(\mathbf{R}_i) + \sum_{j\neq i} G(\mathbf{R}_i, \mathbf{R}_j)d(\mathbf{R}_j)\right],
\]

(4)

where

\[
\alpha = -\frac{D^2}{\hbar[\Delta + i(\gamma + \gamma_0)]}
\]

(5)

is the polarizability of a two-level atom valid at low light intensity. Here \( \gamma_0 \) denotes the HWHM linewidth of homogeneous broadening. Formalism extended to multistate atomic transitions is presented in [11]. The total electric field driving the dipole at the position \( \mathbf{R}_i \) then reads
\[ E(R_i) = E_0(R_i) + \alpha \sum_{j \neq i} G(R_i, R_j)E(R_j). \]  

(6)

Crux of the simulations is to solve numerically such closed inhomogeneous sets of linear equations. The total electric field is then given by

\[ E(r) = E_0(r) + \alpha \sum_j G(r, R_j)E(R_j) \]

(7)

at any field point \( r \) except the positions of the atoms, where the dipolar kernel \( G(r, R_j) \) diverges. Our numerical simulations use the units below

\[ k = \varepsilon = h = \frac{1}{4\pi\varepsilon_0} = 1, \]

(8)

where \( k = 2\pi/\lambda = \omega/c \) is the wavenumber of the incident light with wavelength \( \lambda \). The unit of length is \( k^{-1} \) and the units of quantities related with length are determined accordingly. Unless explicitly mentioned otherwise, all quantities are obtained in these units. We also express the detuning \( \Delta \) and the linewidth of homogeneous broadening \( \gamma_h \) in the unit of linewidth \( \gamma \)

\[ \Delta = \delta\gamma, \]

\[ \gamma_h = \gamma/\gamma. \]

(9)

(10)

Following our conventions, dipole matrix element and the polarizability are given below:

\[ D = \frac{3}{2\sqrt{2}\gamma}, \]

(11)

\[ \alpha = -\frac{3}{2[\delta + i(1 + \gamma_h)]}. \]

(12)

At any field point the magnetic field is

\[ B(r) = -i\nabla \times E(r) \]

(13)

and Poynting vector is

\[ S(r) = \frac{1}{8\pi}[E(r) \times B^* (r)]. \]

(14)

Let us briefly describe setup and quantities to be evaluated in the numerical experiments. The sample embedded into a free space is illuminated by a plane monochromatic light linearly polarized along the \( y \) direction and propagating in the \( z \) direction at normal incidence. Each of 2D square lattices has an interatomic separation \( a \) and lies on the \( xy \) plane with their centers at \( x = -h/2 \) and \( z = h/2 \) such that monolayer lattice is described by the area-number density \( \sigma = a^{-2} \) and the total number of atoms within the bilayer sample is \( 2N \).

Our sample system with \( N = 25 \) is illustrated in figure 1. The primary quantity to be calculated numerically is the optical depth (thickness or density) of the \( 2N \)-atom samples at a far-field point \( r = \xi\hat{e}_z (\xi \geq 1) \) expressed by

\[ D(r) = -\ln T(r) \]

(15)

for the transmittance

\[ T(r) = \left\| \exp(i\xi) + \frac{2\pi\sigma i}{N E_0} \sum_{n=1}^{2N} [d(r_n) - \hat{e}_z \cdot d(r_n)\hat{e}_z] \exp[i(\xi - z_n)] \right\|^2. \]

(16)

Detailed derivations have been given in our previous works [16, 22] and in the other group’s study [30] for different purposes. Equation (16) is obtained in the limit of large lateral size of the 2D planar lattice so that simulation result would be accurate for a sample with a large enough value of \( \sqrt{N}a \) compared with \( a \). Calculation of dipole moments in equation (16) involves a task of finding local fields experienced by atoms at all lattice sites as a backaction to the incident radiation. We then should deal with the dipole propagator which is not absolutely convergent either at small or large interatomic spacing \( a \). Increasing \( a \) from zero, we encounter such a divergence for the first time at \( a = 2\pi \) (\( \lambda \) in SI units) due to Bragg scattering [31]. When nontrivial Bragg scattering is possible for \( a \geq 2\pi \), Bragg scattered waves transport energy to a direction other than the direction of the incident light, leading to energy loss manifesting as \( R(r) + T(r) < 1 \) for the reflectance \( R(r) \). In order to use a relation \( R(r) + T(r) = 1 \) such that there is no energy loss due to Bragg scattered waves, we restrict lattice constants in the range of \( a < 2\pi \) in the present numerical simulations.

3. Two-atom samples

We illustrate the fundamental concepts of light propagation through a two-atom sample by solving equation (6) analytically. For simplicity we do not include the linewidth of homogeneous broadening \( \gamma_h \). We consider the
simplest model in which two atoms positioned at \( z = \pm \frac{h}{2} \) are illuminated by a plane wave linearly polarized in the \( y \) direction and propagating along the \( z \) direction. For the incident light and the positions of the two dipoles
\[
E_0(r) = E_0 \hat{e}_y \exp(iz), \quad r_\pm = \pm \frac{h}{2} \hat{e}_z,
\]
the radiation fields at the positions of two dipoles as solved from equation (6) are
\[
E(r_\pm) = \left[ 1 + \frac{3}{2} \left( \left( \frac{1}{h^3} - \frac{1}{h} \right) \cos h + \frac{\sin h}{h^2} \right) \Delta(h) + \frac{\gamma(h)}{\Delta(h)} \right] E_0 \hat{e}_y \exp \left( \pm \frac{i h}{2} \right).
\]

Here
\[
\Delta(h) = \Delta - \frac{3}{2} \left( \frac{1}{h^3} - \frac{1}{h} \right) \cos h + \frac{\sin h}{h^2} \gamma,
\]
\[
\gamma(h) = \left\{ 1 - \frac{3}{2} \left( \frac{1}{h^3} - \frac{1}{h} \right) \sin h - \frac{\cos h}{h^2} \right\} \gamma.
\]

Equations (19) and (20) manifest themselves as cooperative resonance shift and broadened linewidth of the atoms, respectively, which can be explained as a result of altered vacuum field at the position of one dipole in the vicinity of the other coherently radiating dipole. The modification of vacuum field arises from the light–mediated dipole–dipole interactions owing to repeated exchange of photons between the two atoms, so-called recurrent scattering. Moreover, the \( h \) dependence of cooperative resonance shift \( \Delta(h) \) and linewidth \( \gamma(h) \) evidently reveals the propagation of light from one atom to the other and its effect on cooperative response of atoms. In the limit of \( h \to 0 \) we obtain the shift of the resonance and the linewidth
\[
- \Delta(h) + \Delta \simeq \frac{1.5}{h^3} \gamma, \quad \gamma(h) \simeq 2.0 \gamma.
\]

The shift of the resonance line depends on \( h^{-3} \), which clearly indicates the near-field dipole–dipole interactions between the atoms. On the other hand, the cooperative linewidth is independent of \( h \) and doubles in the small interatomic separation limit. Refer to [22] for analytical calculations of \( \Delta(a) \) and \( \gamma(a) \) in case when two atoms are separated by a distance \( a \) along the direction of the linear light polarization. This suggests that collective resonance shifts and linewidths can be controlled in an aggregation of many cold atoms in different geometries for designing an artificial optical transition [32]. Recent experiment [33] reports cooperative radiation of two neutral atoms strongly coupled to the single-mode field of an optical cavity. Experiment on two trapped ions has also been reported [34]. The expression of dimensionless detuning for which \( \Delta(h) = 0 \) is satisfied reads
\[
\delta_{\text{res}}(h) = \frac{3}{2} \left( \frac{1}{h^3} - \frac{1}{h} \right) \cos h + \frac{\sin h}{h^2}.
\]

At these detunings the radiation field is on the resonance. We use equation (22) as a way to predict detunings for cooperative resonances in numerical simulation of optical spectra.
We also obtain the transmittance and optical depth for the two-atom sample by considering light-induced dipole correlations as follows:

\[ T^{(2)}(\delta, h) = \frac{\delta^4}{\delta^4 + 4(\delta \cos h + \sin h)^2} \]

and

\[ D^{(2)}(\delta, h) = -\ln \left[ \frac{\delta^4}{\delta^4 + 4(\delta \cos h + \sin h)^2} \right] \]

We have provided details for the calculation of equations (A.9) and (A.10) in appendix A. When the two-atom transmittance from equation (23) is plotted as a function of a dimensionless detuning, narrow Fano resonances are observed with a shift corresponding to

\[ \delta_F = -\tan h. \]

The spectral lines are broadened as \( h \) increases in the range of \( \Omega \) and as \( h \) decreases in the range of \( \Omega \). In two different two-atom samples with atomic separations \( h_1 \) and \( h_2 \) under condition of \( h_1 + h_2 = m \pi \) (\( m = 1, 2, 3, \ldots \)), Fano resonances occur at detunings \( \delta = \pm \delta_F \) due to a \( \pi \)-periodicity of tangent function. For example, figure 2 demonstrates the transmittance and optical depth of two-atom samples with \( h_1 = 0.15\pi \) (dashed and solid lines) and \( h_2 = 0.85\pi \) (dotted and dotted–dashed lines), where Fano resonance lineshapes are symmetric around zero detuning. We see that such a behavior is clue for red- and blue-detuned shifts in the spectral response of 3D dense atomic layers to be numerically simulated. Fano resonances in the transmittance correspond to narrow dips in the optical depth at \( \delta_F \). It is evident that lineshapes of optical spectra can be tailored by varying the interatomic distance. In particular, narrow Fano resonances [35] emerge at specific atomic separations. If \( h \) is an integer multiple of \( \pi/2 \) (\( \lambda/4 \) in SI units), the Fano resonances vanish. For an atomic separation a bit smaller or larger than integer multiples of \( \pi/2 \), Fano resonances become sharpest, and transmittances reach almost zero. The similar spectral features for light propagation have been demonstrated for atoms confined in a one-dimensional waveguide [23].

Main feature of a cooperative two-atom response is the modification of optical responses by adjusting the atomic separation; such a feature will be exploited for a collection of cold dense atoms whose optical properties are to be investigated by numerical simulations. For different aspects of cooperativity and ways to control it, refer to [36]. In contrast to the correlated-atom cases, the independent-atom transmittance in the MFT without dipole correlations reads

\[ T^{(2)}_m = \frac{\delta^4}{(\delta^2 + 1)^2} \]

as derived by equation (A.15) in appendix A. Because the repeated photon exchanges between the two atoms are all ignored, the independent-atom transmittance \( T^{(2)}_m \) cannot be modified by varying the interatomic separation. The MFT applies to a many-atom sample of randomly distributed positions at low atomic densities [18].

4. Simulation results

We primarily explore conditions under which an aggregation of homogeneously broadened atoms on a bilayer atomic lattice will cooperatively respond to a driving radiation field using numerical simulation. We focus on a
simple transition \( J_2 = 0 \rightarrow J_2 = 1 \) in the limit of low light intensity such that the classical simulations provide an exact solution for the atomic lattices coupled to the incident radiation.

The dependence of optical depth \( D \) on number density \( \sigma \) of a monolayer lattice within the 2N-atom bilayer samples is represented by a set of graphs of \( D \) as a function of light-emitter detuning \( \delta \), as illustrated in figure 3. Samples under our investigation have a fixed layer-to-layer distance \( h = 0.32 \) and different total numbers of dipoles \( 2N = 162 \) (thin), 578 (dashed), 1058 (red), and 1458 (dotted–dashed). The interatomic separations are set to \( a = \sqrt{256/N} \) such that the monolayer area \( A = Na^2 \) remains constant as 256 (≈6.45\( \lambda_0^2 \)) at the HWHM linewidth of homogeneous broadening \( \gamma_0 = 5.00 \). The criterion \( \sigma \geq 1 \) (\( \sigma k^{-2} \geq 1 \) in SI units), which defines the ‘dense sample’ is satisfied for the cases with \( 2N = 578, 1058, \) and 1458 where respective densities are \( \sigma = 1.13, 2.07, \) and 2.85, while the \( 2N = 162 \) sample with \( \sigma = 0.32 \) is not. It is evident that three-dimensional (3D) lattice geometry formed by two planar lattices gives rise to optical responses of emitters that are quite different from those for 2D lattices [16, 17], and significantly modifies absorption line shapes at special sample parameters. First, we find that cooperative resonance shifts of the bilayer atomic lattices are exhibited both at positive and negative detunings as already demonstrated in figure 2 for the two-atom cases. On the other hand, resonance lines from monolayer square lattices [16] were shifted only to negative detunings, which is plotted as a gray line in figure 3 for a \( N = 1024 \) monolayer lattice of \( a = 0.71 \). Secondly, cooperative resonance shifts of the bilayer lattices, which for monolayer lattices are proportional to the atomic density \( \sigma \), are reduced as \( \sigma \) increases; the bilayer lattice of \( 2N = 1458 \) atoms exhibits least resonance shift as shown in figure 3. Such an aspect is seemingly against the fact that the size of shift is proportional to the area density; this may be interpreted as an outcome of a cooperative optical response. Therefore, a 3D lattice structure might be used for the elimination of resonance shifts, which is crucial in order to improve spectroscopic accuracy in 3D optical lattice clocks [37]. Moreover, enhanced optical response of the bilayer samples is distinctly shown in comparison of the 1024-atom monolayer plot with the 1058-atom bilayer one; a pair of identical N-atom planar lattices with the same number density \( \sigma \) exhibits greater maximum values and linewidths of optical spectrum than for a monolayer lattice of \( 2N \) atoms with the same \( \sigma \). We emphasize such enhanced responses of the bilayer samples furthermore by presenting analytical expression of the optical depth for a planar lattice of independent 1024 atoms:

\[
D = \frac{6\pi}{a^2(\delta^2 + 1)}
\]  

(27)

plotted as a dotted line in figure 3. Equation (27) is obtained from independent-dipole scattering theory [7] that does not include dipole–dipole interactions of the planar lattice. In homogeneously broadened samples in figure 3, correlations between the dipoles are important and for these samples interactions between dipoles are cooperative. Such correlations originate from a recurrent scattering of photons between atoms, because each of sample atoms has the same resonance frequency.

We also find two resonances of the absorption line in figure 3. As the total number of atoms is increased so that the number density of monolayer lattice is increased, resonant optical thicknesses of the samples are strengthened with their increased linewidths, and two peaks are placed closer: the separations between two resonance lines are 92.4, 86.8, 77.6, and 70.0 in our unit of frequency for the samples of \( 2N = 162, 578, 1058, \) and 1458, respectively. Number and density dependence of linewidths manifest itself and they are proportional to a degree of cooperative optical responses of the atoms, which arises from all the repeated photon exchanges between the sample atoms. Cooperative linewidths are modified by varying the total number of atoms and lattice
constant such that a collective superradiant or subradiant [38–40] emission can be engineered in a pair of planar atomic lattices in the optical frequency domain.

We understand that two resonances are reminiscent of Fano resonances of optical depth illustrated in figure 2 as dips for a two-atom sample. Such resonance shifts on the absorption line manifest themselves as a cooperative feature [15] that cannot be predicted by equation (B.1) in appendix B from an EDPM. They are attributed to collective resonance shifts $\Delta_\alpha h$ associated with two collective linewidths $\Gamma_\alpha$, which originate from imaginary part of the sum over left- and right-propagating fields along the $\pm z$ directions from one lattice plane to the other and vacuum field. Therefore, in the far-field sample dipoles radiatively decay into three modes: left- and right-propagating modes and vacuum mode. Markedly different broadenings of the optical spectra at different interatomic and interlayer separations where the ratio $\Delta_\alpha h$ to $\Gamma_\alpha h$ varies at different layer-to-layer distance $h$. Evidently, both resonance shifts and radiative decay rates of many-atom sample can be tailored by adjusting spatial arrangement of atoms. An analogous phenomenon, which exhibits two resonances in the absorption spectrum as sample atomic density varies, has been displayed in the monolayer kagome lattices in the previous work [16]. Presumably, two collective modes corresponding to left- and right-propagating modes for the bilayer lattices arise from two emitters of different dipole moments as for the case with each primitive unit cell of kagome lattice. We surmise that bilayer atomic lattices are two effective superatoms separated by the propagation direction of incident radiation. Similar superatom model [41] for a planar lattice of atoms is used to understand light propagation through stacks of planar lattices. Numerical resonance shifts are in good agreement with analytical results from an infinite and isotropic lattice model which has been introduced for calculating resonance shift of monolayer lattices [16]. We will present detailed and quantitative analysis regarding superatom analogy with bilayer atomic lattice.

We discuss dependence of resonance shifts and line shapes on interatomic and interlayer separations. The absorption line shape is altered significantly by varying $h$ alone and keeping $a$ and $2N$ fixed as shown in figure 4, where $h = 0.25$ (gray line), 1.00 (dotted), and 2.00 (blue) are used for bilayer square lattices with $a = 1.00$ and $2N = 1058$ atoms. Such a feature is also a cooperative effect that has no parallels in EDPM, because according to equation (8.1) in appendix B, it is absolutely impossible to modify a shift of the resonance line by varying interlayer distance alone. Relatively large lattice constants within $h = 1.00$ and $h = 2.00$ samples allow the dipoles on the front layer to interact weakly with those on the back, leading to the absence of second peak and narrower line shapes. In particular, relative phases of the periodically ordered dipoles within a pair of square lattices give rise to large Bragg reflection such that above 99% reflectances are exhibited for $h = 1.00$ and $h = 2.00$ samples at nearly $\delta \approx 0$. At particular lattice constants satisfying conditions for zero transmittance, radiation incident to the samples at exact atomic resonance frequency is completely reflected. Such a resonant suppression of the transmission is the main feature of the Fano resonance [35], and similar characteristic 2D features were obtained for 2D arrays of resonant ultracold atoms loaded into optical lattices [21] and of artificial atoms in the solid-state context [13]. Further numerical simulations reveal that the absorption line is not split into two in a regime of interlayer separation $h \gtrsim 0.25 \pi$ for samples used in figures 3 and 4. This is reasonable, because dipoles are more weakly correlated in this regime than in the opposite regime for $h$. Therefore, to a good approximation, optical responses of the bilayer atomic lattices with $h \gtrsim 0.25 \pi$ used in figures 3 and 4 can be explained by standard optics.

We now further investigate effects of the interlayer separation on the absorption line shape. Figure 5 shows maximum values of the optical depth of a 512-atom bilayer sample as a function of interlayer separation $h$ for lattice constants $a = 0.870$ (cross), 1.00 (circle), $\sqrt{2}0.00$ (gray), and 1.10 (black). We collect maximum values of the optical depth from the plots of $D$ versus $\delta$ for various interlayer separations at each of four lattice constants.

Figure 4. Optical depth $D$ of $2N = 1058$ bilayer lattices with atomic separation $a = 1.00$ versus light-emitter detuning $\delta$. Layer-to-layer distances are $h = 0.25$ (gray line), 1.00 (dotted), and 2.00 (blue), respectively.
To validate simulation schemes, we compare the results for $a = \sqrt{2.00}$ and $1.10 \pi$ with analytical approximation by modeling each monolayer lattice as a single superatom acting as a mirror with the amplitude reflection and transmission coefficients $r_i$ and $t_i$ $(i = 1, 2)$. From the Fabry–Pérot transmittance, the corresponding optical depth reads

$$D = -\ln \left( \frac{t_1 t_2}{1 - \eta r_2 \exp(i2h)} \right)^2. \quad (28)$$

Analytical calculations of optical depth from equation (28) are shown as dashed and dotted lines for $a = \sqrt{2.00}$ and $1.10 \pi$ in figure 5. The simulation result for $a = \sqrt{2.00}$ is plotted as a gray line and coefficients $t_1 = t_2 = 45.0\%$ and $r_1 = r_2 = 55.0\%$ are used to fit the simulation. A black line in the bottom shows the simulation result for $a = 1.10 \pi$ with fitted coefficients $t_1 = t_2 = 86.4\%$ and $r_1 = r_2 = 13.6\%$. Exact calculations of $r_{1(2)}$ and $t_{1(2)}$ using quantum-mechanical framework have been presented in [27], where a pair of two-level atoms within a one-dimensional (1D) waveguide is considered as a model system. Deviation from numerical simulation is substantial for a small $h (\approx \pi)$ as shown in figure 5, while it is negligible for a large $h (\gg \pi)$. Such a deviation is plausible because dipoles are strongly correlated in the limit of $h \to 0$ than in the one of $h \to \infty$. For two dilute samples with $a = \sqrt{2.00}$ and $1.1 \pi$, sinusoidal behavior of optical spectra with a $\pi$-periodicity qualitatively agrees with results for an optical cavity-like system, which is predicted by standard optics. This spatial periodicity of absorption spectrum is also exhibited for samples with lattice constants $a \gtrsim 1.1 \pi$. On the other hand, as demonstrated in figure 5, dense samples interact with light quite differently in that peaks of the sample with $a = 1.00$ are split into two at $h = \frac{\pi}{2}, \frac{3\pi}{2}, \frac{5\pi}{2}$, and the optical depth is abruptly increased by varying interlayer separation slightly from $h \approx 9.82 \lambda_0$ ($1.56\lambda_0$) to $h \approx 10.0 \lambda_0$ ($1.59\lambda_0$). Similar splitting of the peaks and abrupt changes in optical depth are also observed for the sample with $a = 0.860$ at different $h$. In particular, the transmittances are almost zero at interlayer distances for which peak values of the optical depth are obtained so that periodic occurrences of zero transmittances are displayed by varying the interlayer separation of the bilayer lattice. Presumably, optical spectra of our bilayer atomic lattices are tailored by adjusting the lattice parameters. For example, tailored transmittance at proper lattice constant $a \lesssim 2 \pi$ and interlayer separation $h$ may be used to implement on- and off-states for a high-fidelity logic gate in quantum computing.

The similar theoretical findings were reported earlier on an array of resonant dipoles in the solid-state context [13] and for the light propagation through a triangular 2D array of $N = 102$ interacting atoms [17]. More theoretical investigations of 2D lattice samples of atoms interacting with light can be found in [13, 21, 24, 42, 43]. Refer to [44] and references therein for recent theories on plasmonic nanoparticles formed by 2D planar lattices.

One of candidate systems to realize our numerical simulation scheme experimentally is an optical lattice in a Mott-insulator state in which the atomic positions in each site fluctuate due to the vacuum fluctuations in the ground state. These atomic position fluctuations vary depending on the confinement strength of the atoms to the optical lattice potential. The greater the confinement strength is, the less the position fluctuations are anticipated. In large-scale simulations of homogeneously broadened atomic gases, we should not neglect the effects of the atomic position fluctuations on the optical spectra to be measured. However, realistic large-scale simulations require longer computation time, because we need to compute the ensemble averages after stochastically sampling the positions of atoms in each individual 2D lattice site from a position distribution of interest. Therefore, we consider a case of tight confinement of atoms to the optical lattice. The effects of the fluctuations of the atomic positions was recently investigated for the numerical simulations of an array of atoms in a 1D waveguide [23]. The other experimental issue to be resolved is to reduce photon loss, which may be substantially reduced in atoms confined in a photonic crystal [45].
5. Conclusion

We have discussed that cooperative response is a fundamental concept of light propagation through a pair of identical 2D square lattices of homogeneously broadened dense atoms. Cooperativity originates from light-induced strong correlation between atoms and its major application predicted is the modification of optical spectra by adjusting lattice constant and interlayer distance of the bilayer lattices. In particular, bilayer atomic lattices could be manipulated such that they reflect all of a driving radiation field at properly selected lattice parameters and cancel density-dependent resonance shifts at specific polarization and propagation direction of the probing light. We semiclassically perform numerical simulations of steady-state point-like dipoles within a nanometer-scale sample coupled to low-intensity light by solving the coupled-dipole equation. We elucidate that there exists a strongly correlated regime of sample parameters in which cooperative phenomena occur. In the other regimes, positions and dipole moments of the atoms are weakly correlated so that analysis from standard optics can explain collective behaviors of the samples. One instance is to use the Fabry–Pérot transmittance to explain plots of optical depth as a function of interlayer separation in the low-density regime using the superatom analogy of the bilayer lattices. In the strongly correlated regime, simulation results are in qualitative agreement with predictions from an isotropic infinite lattice model. Nonetheless, there remains hosts of cooperative features yet to be explained both from a new electrodynamics theory pertinent to nanometric samples and a phenomenological method using large-scale numerical simulations.

A bilayer atomic lattice might be exploited to engineer collective resonance shifts, HWHM linewidths of the optical transition, and transmittances by tuning system parameters. Such a lattice could find applications in on- and off-states for an optical switch and a photonic device. Numerical simulations with computer clusters for total number of atoms as large as 140 000 will shed lights on this issue.

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Appendix A. Analytical optical spectra for a two-atom sample

In appendix A we derive optical spectra for a two-atom sample as shown in equations (23)–(26) using the transfer matrix method originating from the Fresnel equations [46]. We follow a formalism [23] previously introduced for light propagation through an array of cold atoms confined in a 1D waveguide. Here we do not consider radiative losses out of the sample. The slowly varying picture has been used to describe the time-dependent classical quantities, so $\tilde{E}^+$ denotes the positive frequency component of electric field. For a coupled sample of light traveling along the $+z$-direction and a single point-like atom positioned at $z_1$, the transmission amplitude $\tilde{E}^+_t$ in the region of $z > z_1$ is obtained in terms of the incident and reflected field amplitudes $\tilde{E}^+_i$ and $\tilde{E}^-_r$ in $z < z_1$ as follows:

$$
\begin{pmatrix}
0 \\
\tilde{E}^-_t
\end{pmatrix}
= T(\Delta)
\begin{pmatrix}
\tilde{E}^+_i \\
\tilde{E}^-_r
\end{pmatrix}
$$

(A.1)

Here a transfer matrix $T$ as a function of detuning $\Delta$ reads

$$
T(\Delta) = \begin{pmatrix}
\frac{i\Delta - \gamma}{i\Delta} & -\frac{\gamma}{i\Delta} \\
\frac{i\Delta}{\gamma} & \frac{i\Delta}{i\Delta + \gamma}
\end{pmatrix}
$$

(A.2)
The transmission and reflection amplitudes are respectively obtained as
\[ t^{(1)}(\Delta) = \frac{\hat{E}_t^+}{\hat{E}_i^+} = \frac{i\Delta}{i\Delta - \gamma}, \]
\[ r^{(1)}(\Delta) = \frac{\hat{E}_r^+}{\hat{E}_i^+} = \frac{\gamma}{i\Delta - \gamma}. \]

For two identical atoms placed at \( z_1 \) and \( z_2 \) we should consider the propagation phases of the light from \( z_i \) to \( z_{i+1} \), which is expressed by the matrix
\[ \phi(z_{i+1}, z_i) = \begin{pmatrix} \exp[i(z_{i+1} - z_i)] & 0 \\ 0 & \exp[-i(z_{i+1} - z_i)] \end{pmatrix}. \] (A.5)

Two positions to the left and to the right of the two-atom sample are denoted by \( z_0 \) and \( z_3 \), and a composite transfer matrix \( T_{03} \) is
\[ T_{03} = \phi(z_3, z_2)T(\Delta)\phi(z_2, z_1)T(\Delta)\phi(z_1, z_0). \] (A.6)

The incident and reflected amplitudes are then described by
\[ \begin{pmatrix} 0 \\ \hat{E}_r^+ \end{pmatrix} = T_{03} \begin{pmatrix} \hat{E}_i^+ \\ 0 \end{pmatrix}. \] (A.7)

The transmission amplitude is then
\[ t^{(2)} = \frac{\Delta^2 \exp[i(z_1 - z_0)]}{\gamma^2 \exp(2i\hbar) - (i\Delta - \gamma)^2}. \] (A.8)

It would be worth addressing what the expression for \( t^{(2)} \) implies: \( \exp(2i\hbar) \) (with \( \hbar = z_2 - z_1 \)) in the denominator is a propagation phase for a single oscillation of the light between the positions of atoms 1 and 2.

From the double-angle identities of trigonometry, we obtain the two-atom transmittance and optical depth:
\[ T^{(2)}(\delta, h) = |t^{(2)}|^2 = \frac{\delta^4}{\delta^4 + 4(\delta \cos h + \sin h)^2}, \]
\[ D^{(2)}(\delta, h) = -\ln T^{(2)} = -\ln \left[ \frac{\delta^4}{\delta^4 + 4(\delta \cos h + \sin h)^2} \right]. \] (A.9) (A.10)

Resonance of the transmittance in equation (A.9) occurs at a particular detuning \( \delta_F \) expressed by
\[ \delta_F = -\tan h. \] (A.11)

At the detuning \( \delta = \delta_F \) the two-atom transmittance equals 1. In a case when the linewidth of homogeneous broadening is included, we obtain
\[ T^{(2)}(\delta, \gamma_h, h) = \frac{\delta^4}{\delta^4 + 4(1 + \gamma_h^2)(\delta \cos h + (1 + \gamma_h)\sin h)^2}, \] (A.12)
from which resonance detuning is given by
\[ \delta_F = -(1 + \gamma_h)\tan h. \] (A.13)

Finally, if light-induced correlations are neglected, each atom in the sample conveys the same amount of light. Then the MFT two-atom transmission amplitude \( t^{(2)}_m \) would be constructed by the product of the single-atom transmission amplitudes equation (A.3):
\[ t^{(2)}_m = t^{(1)}_1 t^{(1)}_2 = \frac{\delta^2}{\delta^2 - 1 + 2i\delta}. \] (A.14)

We then obtain the MFT transmittance
\[ T^{(2)}_m(\delta) = \frac{\delta^4}{(\delta^2 + 1)^2}. \] (A.15)

For nonzero linewidth of homogeneous broadening we obtain
\[ T^{(2)}_m(\delta, \gamma_h) = \frac{\delta^4}{[\delta^2 + (1 + \gamma_h^2)]^2}. \] (A.16)

Note that the MFT optical spectra may be valid in the limit of low density for atomic ensembles with stochastically distributed positions.
Appendix B. Electrodynamics of a bilayer of dielectrics

If light is normally incident from free space to the double identical slabs of depth $d$ and the index of refraction $n$, which are separated by distance $h$, the optical depth calculated from standard optics [46] reads

$$D = -\ln \left| \frac{8n^2}{f(d, h)} \right|^2,$$

where $f(d, h) = 2n(n + 1)^2 \cos(2nd + h) - 2n(n - 1)^2 \cos(2nd - h) - i[(n^2 + 1)(n + 1)^2 \sin(2nd + h) - 2(n^2 - 1)^2 \sin h] + i(n^2 + 1)(n - 1)^2 \sin(2nd - h)$.

EDPM introduces the local-field corrections so that all atoms see the effective field, leading to the refraction index of the slabs with the same number density $\rho$ written as

$$n^2 = 1 + \frac{D^2 \rho}{\Delta + 2\pi \rho + \gamma}.$$  \hspace{1cm} (B.2)

Even if this analytical result cannot be exactly applied to samples in our numerical simulation because of zero field corrections so that all atoms see the effective field, clearly, standard optics predicts that absorption lineshape has one peak and resonance lines are shifted only to negative detunings. Furthermore, we can figure out the interferences of light propagating along six different paths within a bilayer sample from the denominator of equation (B.1).

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