Coexistence of Surface Lattice Resonances and Bound states In the Continuum in a Plasmonic Lattice

Quoc Trung Trinh¹, Sy Khiem Nguyen¹, Dinh Hai Nguyen¹, Gia Khanh Tran¹, Viet Hoang Le¹, Hai-Son Nguyen²,³, and Quynh Le-Van¹∗

¹College of Engineering and Computer Science, VinUniversity, Gia Lam district, Hanoi 14000, Vietnam
²Univ Lyon, Ecole Centrale de Lyon, CNRS, INSA Lyon, Université Claude Bernard Lyon 1, CPE Lyon, CNRS, INL, UMR5270, 69130 Ecully, France and
³Institut Universitaire de France (IUF), Paris, France

(Dated: March 29, 2022)

We present a numerical study on a 2D array of plasmonic structures covered by a subwavelength film. We explain the origin of surface lattice resonances (SLRs) using coupled dipole approximation and show that the diffraction-assisted plasmonic resonances and formation of bound states in the continuum (BICs) can be controlled by altering the optical environment. Our study shows that when the refractive index contrast ∆n > 0.1, the SLR cannot be excited, while a significant contrast (∆n > 0.3) not only sustains plasmonic-induced resonances but also forms both symmetry-protected and accidental BICs. The results can aid the streamlined design of plasmonic lattices in studies on light–matter interactions and applications in biosensors and optoelectronic devices.

Surface lattice resonances (SLRs) are delocalized modes emerging as localized surface plasmon resonances (LSPRs) of individual plasmonic particles that are radiatively coupled to the diffraction orders of the incident light waves induced by the lattices [1, 2]. The lattice mode is also studied in lossless systems [3]. The coupling is a mechanism to mitigate the ohmic losses from the LSPRs to the diffracted waves. As a result, SLRs are characterized by an increased quality factor over LSPRs and by a sharper Fano resonance in the scattering spectra [4–6]. These remarkable properties have attracted significant interest for potential applications in lasers [7–9], strong light-matter interactions [10, 11], nonlinear optics [12], and biosensors [13]. Another peculiar aspect of Fano resonances is their disappearance in the scattering spectra. The collapse of Fano resonances is a signature of the bound state in the continuum (BIC) [14, 15]. This disappearance leads to an infinite Q-factor and has been experimentally proven in dielectric systems [16–18]. Recently, several groups have theoretically proposed [19–24] and reported the BICs in lossy media [25–27]. Interestingly, both SLRs and BICs can be realized in periodic structures despite having opposite features in terms of the Fano resonances. To date, there has been no report on any plasmonic system that supports both SLRs and BICs. Here, we propose a simple plasmonic structure made of a silver nanodisks array that can host both SLRs and BICs simultaneously. We elaborate on the physics of the system through numerical studies under varied conditions of the excitation angle, periodicity, and refractive index of the covered layer. We show that three distinct regions with different physics can be obtained for the given system.

We begin our study by addressing the origin of the SLRs in a 2D square lattice at normal incidence. Our system comprises an array of silver nanodisks (radius $r = 40$ nm and height $h = 40$ nm) with periodicity $p$, as illustrated in Fig. 1a. They are placed on a glass substrate ($n_{sub} = 1.46$) and covered by a 200 nm thick superstrate with refractive index $n_{sup}$. We used the coupled dipole approximation (CDA) to calculate the spectral positions of LSPRs, Rayleigh anomalies, and SLRs [28]. In this framework, when a periodic array of identical subwavelength nanoparticles is impinged by an external plane wave, each particle can be characterized as an electric dipole with polarizability $α_E$ [29] and subjected to the total applied fields, including the incident waves and retarded fields by the neighboring particles. Thus, the effective polarizability $α$ of each particle is given by $α^{-1} = α_E^{-1} − S$ [30]. Here $S$ is the lattice sum describing the dipole coupling mechanisms between a particle and its neighbors. Note that $α_E$ and $S$ are complex values due to the presence of Ohmic and radiative losses. In addition to dipole interactions, the diffraction of the periodic array is another pronounced effect in response to the incident waves. The diffracted waves can radiate in the regions above, possibly below, and in the array. An interesting physical phenomena occur as the wave diffracts in the plane of the array, known as Rayleigh anomaly. The corresponding condition for such an effect is the zero-propagation constant in the propagation direction. In other words, the condition for Rayleigh anomalies in the Cartesian system is given by $ε_r = \left(\sin θ \cos Φ + \frac{1}{p}\right)^2 + \left(\sin θ \sin Φ + \frac{n}{p}\right)^2$ where the pair $(m,n)$ corresponds to the diffraction orders, and $θ$ and $Φ$ are the incident and azimuthal angle, respectively (see Fig. 1a). The far-field reflectance for normal incidence can be expressed as $R = \left|\frac{P}{P_0}\right|^2$ [28, 31], leading to photonic resonances at the zeros of the real part of $α^{-1}$. Figure 1b shows the calculated $ℜ(α_E^{-1})$ and real values of the lattice sum $S_1$ and $S_2$ corresponding to two periods $p_1 = 325$ nm and $p_2 = 425$ nm. The $ℜ(S_1)$ value is low, indicating a modest contribution of the lattice in the

* quynh.lv@vinuni.edu.vn
α polarizability (1/Å²).

A square lattice of silver nanodisks on a substrate (r = h = 40 nm) and lattice sums S₁ of p₁ = 325 nm and S₂ of p₂ = 425 nm at θ = 0°. Simulated reflectances at θ = 0° of the structures with n_{sup} = 1.5. Three peaks in c) agree well with the crossing points in b). The electric fields of peaks: A (d-e), B (f-g) and C (h-i) for a unit cell. The orange dash lines indicate the interfaces between layers.

First, the intersection with the sharp drop (2.0 eV) corresponds to the diffracted waves or Rayleigh anomaly. The crossing at 1.95 eV (635.9 nm) and 2.33 eV (532.1 nm) are signatures of the SLR and LSPR, respectively. To verify the predictions, we performed a numerical simulation of the scattering spectra for such geometries using Comsol Multiphysics with TE polarization and Floquet boundary conditions. Figure 1c shows the simulated electric field in y-direction for three resonances: SLR (1.72 eV), GR (1.92 eV), and LSPR (2.02 eV). Figure 2c presents the calculated electric field in y-direction for three resonances, the lattice. b) Truncated spectra at specific values in Fig. 2a. c) Calculated electric field in y-direction for three resonances as a function of z position for Δn = 0.34. d), e) Electric field of GR.

FIG. 2. Excitations of the SLR with varying refractive index contrast. a) Evolution of the resonances in the index contrast Δn = -0.46−0.94. Three regions (I, II, and III) are observed. The numbers in parentheses indicate the diffracted orders of the lattice. b) Truncated spectra at specific values in Fig. 2a. c) Calculated electric field in y-direction for three resonances as a function of z position for Δn = 0.34. d), e) Electric field of GR.

spectral range. In contrast, the \( \Re(S_2) \) shows an abrupt drop to zero-value at 2.0 eV. The intersection of \( \Re(\alpha_E^{-1}) \) with \( \Re(S_1) \) is evidence of an LSPR, whereas it crosses \( \Re(S_2) \) at three distinct values.

We investigated the role of the superstrate for the nanodisk array with a period p = 425 nm in sustaining both LSPRs and SLRs. n_{sup} is varied from 1.0 (air) to 2.4 (TiO₂ [32] or perovskite film [33, 34]). This corresponds to a variation in the index contrast, defined by \( Δn = n_{sup} - n_{sub} \), from -0.46 to 0.94. Although SLRs have been studied in inhomogeneous media [35], only low index contrast (≤9%) was considered. Here, the contrast range was extended up to 64% (Δn = 0.94). Figure 2a shows three regions with distinct features: the region I, Δn < -0.1, which only supports the LSPR because the waves propagate in the superstrate owing to its higher refractive index. Region II supports both LSPR and SLR as the index contrast is kept at a minimum (-0.1 < Δn < 0.3). Notably, an additional sharp peak appears in the region III (Δn > 0.3) between the LSPR and SLR. This sharp resonance is attributed to a guided resonance (GR) [36–38] which is a dielectric guided mode confined within the superstrate and is diffracted into the radiative continuum owing to the lattice effect. Naturally, this GR is less exposed to the nonradiative losses of the metallic particles than the LSPR and SLR, thus, it would exhibit much higher Q-factors. To verify the nature of the resonances, we truncated the spectra at three representative values for each region (see Fig. 2b). The spectrum when Δn = 0.34 exhibits two distinct peaks, (LSPR and SLR) as shown in Fig. 1c. Lastly, the spectrum for Δn = 0.34 reveals three peaks: LSPR (1.72 eV), GR (1.92 eV), and LSPR (2.02 eV). Figure 2c presents the calculated electric field in y-direction for the resonances. As expected, the SLR field is maximum in the lattice plane, whereas the GR field is maximum at the boundary between the superstrate and the air. However, the GR field also exhibits a local maximum near the plasmonic particle. This suggests that this GR is resulted from the hybridization between pure guided mode and LSPR. Figures 2d and e confirm this...
branch has a pronounced resonance signal at the Γ point. SLR branch fades closer to the Γ point and is not visible. Notably, under such a large index contrast the enhanced coupling between the LSPR and Rayleigh approaches the diffraction line. This can be attributed to observe that the SLR becomes sharper as the periodicity of the band diagram as the periodicity is tuned. We also in the frequency of the LSPR results from the reshaping the materials and the optical environment. The change contrasts, which are presented in Figs. 3a and 3b, respectively. As shown in Fig. 3a, the LSPR frequency decreases with increasing periodicity. This contradicts the common belief that the frequency is solely determined by the materials and the optical environment. The change in the frequency of the LSPR results from the reshaping of the band diagram as the periodicity is tuned. We also observe that the SLR becomes sharper as the periodicity approaches the diffraction line. This can be attributed to the enhanced coupling between the LSPR and Rayleigh anomalies. Notably, under such a large index contrast ∆n = 0.34, the GR is not always excited. Instead, the GR is excited when it couples with the LSPRs. As a result, the losses of the LSPR are alleviated via hybridization with the GR, and hence, the Q-factors of these LSPRs significantly increase. Conversely, the Q-factors of the SLRs deteriorate owing to reduced coupling with the in-plane diffractions. We analyzed the angle dependence of the SLRs when excited in a quasi-homogeneous environment, ∆n = 0.04. As they are probed in wavevector kx (Fig. 4a), their optical responses are shaped by the coupling between the LSPR and the diffraction orders (±1,0). The LSPR in Figs. 4a and b exhibits relatively constant energy when excited from oblique angles. In contrast, the SLRs emerging from the coupling between the LSPR and the diffraction order (±1,0) show strong angular dependence. Two SLR branches can be observed along kx, both exhibiting a linear dispersion as they approach the diffraction order (±1,0). The upper SLR branch fades closer to the Γ point and is not visible at normal incidence. In comparison, the lower SLR branch has a pronounced resonance signal at the Γ point and fades at oblique angles. When probed in ky, only the lower SLR branch is visible with a quadratic dispersion, closely following the characteristics of the diffraction order (0,±1). We note that changing polarization and fixing the probe angle will produce the same results as a fixed polarization and changing probing directions as in this work. Figure 4c presents the Q-factors of the different SLR branches plotted as a function of the wavevector. As kx deviates from the Γ point, the Q-factor increases rapidly for the SLR branch (-1,0) and reaches a plateau (Q = 300) when fading to the Rayleigh anomalies (kx > 1µm⁻¹).

Finally, we investigated the angle-resolved response of the structure with a high-index contrast ∆n = 0.34. As shown in Fig. 5, we find strikingly different responses compared with the low-index contrast case, as shown in Fig. 4. First, the LSPR and lower SLR bands are reshaped by the contraction of the band diagram owing to the change in the refractive index. This leads to a quadratic dispersion of the LSPR bands. More importantly, three GR-like bands with a high curvature emerged between the LSPR and lower SLR bands. The highest energy band corresponds to the one denoted as GR in our previous studies (Figs. 2 and 3), resulting from the hybridization between a pure GR and the LSPR. Here, the angular-resolved reflectance of this band reveals that it gets sharper when moving away from the G point and eventually reaches its highest quality factor at kx = 0.78 µm⁻¹ and E = 1.925 eV (Δ = 675.3 nm) when its scattering resonance vanishes locally in the momentum space, see Fig. 5b. Such behaviors are the hallmarks of an accidental BIC (a-BIC) that occurs when the hybridization mechanism leads to a destructive inter-

FIG. 3. The reflectance of the system (at θ = 0°) with tuned periodicity for two refractive index contrasts. a) ∆n = 0.04 and b) ∆n = 0.34. The dash curves with numbers in parentheses are diffraction orders of the lattice.

FIG. 4. Angle-resolved reflectance of the silver nanodisk array for ∆n = 0.04 and p = 425 nm. The reflectance is probed a) in kx and b) in ky. c) Q-factor of different bands of SLRs. d) Spectra truncated in a) and b) at θ = 0° and θ = 6°. The solid and dashed lines are associated with the spectra probed in kx and ky, respectively.
ference configuration [39]. On the other hand, the spec-

tral range and curvature of the second and third GR-
like bands suggest that they are hybridizations between
a pure GR and the upper SLR branch depicted in Fig.
5a. Moreover, because the upper SLR branch does not
exist in the vicinity of the Γ points (i.e. \(|k_x| < 0.1 \mu m^{-1}\),
Fig. 5a), these two bands are of a GR nature solely
in this range. Interestingly, their scattering resonances
vanish at the Γ point when energies \(E = 1.845 \text{ eV} (\Lambda =
672 \text{ nm})\) and \(1.836 \text{ eV} (\Lambda = 675.3 \text{ nm})\), while becoming
broader as soon as they are under oblique excitation.
Therefore, they are symmetry-protected BICs (s-
BICs), in which the coupling to the radiative continuum
is strictly forbidden owing to the \(C_4\) symmetry mismatch
between their in-plane pattern and the radiating plane
waves [39]. Magnified views of the a-BIC and the two s-
BICs are presented in the upper and lower panels of Fig.
5c. Figure 5d depicts the electric field distributions of the
three BIC states, confirming that the a-BIC is indeed of a
hybrid GR–LSMR nature, while the two s-BICs are solely
of a GR nature. We used the Q-factor to compare these
BICs with others reported for plasmonic systems. The
Q-factors in our system reached remarkably high values
(\(\sim 10^4\)) in the BIC states, as shown in Fig. 5b. We
note that in plasmonic systems, the Q-factor is bounded
by the nonradiative losses from the metallic component,
and most of the reported BICs from plasmonic systems
designed for infrared and visible frequencies exhibit Q-
 factors only in the range of \(10^2 \sim 10^3\) [20, 26, 27].
Our results show that by using GR-like modes, the lossy flaw
in plasmonic systems can be mitigated, thus providing
ultra-high-quality factors even with metallic components.
A similar result was recently reported for 1D plasmonic gratings [40].

In conclusion, we demonstrated that plasmonic structures
can enable a variation in the resonance as well
as in the trapped light in the form of BICs. The key
constraint to unlock this interesting phenomenon is the
large refractive index contrast surrounding the plasmonic
particles. Our study demonstrated a new application of
guided resonance as an effective mechanism to mitigate
the absorptive losses of the plasmonic particles and
revealed that the waveguide effect can lead to the
formation of BICs in a lossy medium. The findings
could be implemented in plasmonic lattice covered by
a thin film of perovskite or semiconductor nanocrystals
for applications in sensing and light-emitting devices.

Funding Information This work was funded
by Vingroup Big Data Institute, Vingroup
VINIF.2021.DA00169.

Acknowledgement. Q. L-V would like to thank
Bojorn Maes for his critical assistance with simulation
models.

Disclosures. The authors declare no conflicts of inter-

[1] S. Zou, N. Janel, and G. C. Schatz, Silver nanoparticle
array structures that produce remarkably narrow plas-
mon lineshapes, The Journal of Chemical Physics 120,
10871 (2004), https://doi.org/10.1063/1.1760740.
[2] V. A. Markel, Divergence of dipole sums and the nature
of non-lorentzian exponentially narrow resonances in one-
dimensional periodic arrays of nanospheres, Journal of
Physics B: Atomic, Molecular and Optical Physics 38,
L115 (2005).
[3] V. E. Babicheva and A. B. Evlyukhin, Reso-
nant lattice kerker effect in metasurfaces with
electric and magnetic optical responses, Laser
& Photonics Reviews 11, 1700132 (2017),
https://onlinelibrary.wiley.com/doi/pdf/10.1002/lpor.201700132.
[4] A. E. Miroshnichenko, S. Flach, and Y. S. Kivshar, Fano
resonances in nanoscale structures, Rev. Mod. Phys. 82,
2257 (2010).
[5] Q. Le-Van, E. Zoethout, E.-J. Geluk, M. Ramezani,
M. Berghuis, and J. Gómez Rivas, Enhanced
quality factors of surface lattice resonances in
plasmonic arrays of nanoparticles, Advanced
Optical Materials 7, 1801451 (2019),
https://onlinelibrary.wiley.com/doi/pdf/10.1002/adom.201801451.
[6] M. S. Bin-Alam, O. Reshef, Y. Mamchur, M. Z. Alam,
[39] C. W. Hsu, B. Zhen, A. D. Stone, J. D. Joannopoulos, and M. Soljačić, Bound states in the continuum, Nature Reviews Materials 1, 16048 (2016).

[40] Z.-L. Deng, F.-J. Li, H. Li, X. Li, and A. Alù, Perfect diffraction metagratings supporting bound states in the continuum and exceptional points, arXiv, 2109.10533 (2021).

[41] W. L. Barnes, Particle plasmons: Why shape matters, American Journal of Physics 84, 593 (2016).

[42] B. Špačková and J. Homola, Sensing properties of lattice resonances of 2d metal nanoparticle arrays: An analytical model, Opt. Express 21, 27490 (2013).