Kerker Condition for Enhancing Emission Rate and Directivity of Single Emitter Coupled to Dielectric Metasurfaces

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Metasurfaces have the ability to control classical and non-classical states of light to achieve controlled emission even at the level of a single emitter. Here, the Kerker condition induced emission rate enhancement with strong directivity is unveiled from a single emitter integrated within a dielectric metasurface consisting of silicon nano-disks. The simulation and analytical calculations attest the Kerker condition with unidirectional light scattering evolved by the constructive interference between electric dipole, toroidal dipole, and the magnetic quadrupole. The results evince spatially-dependent enhanced local density of optical states, which reciprocates localized field intensity. The emission rate enhancement of 400 times is achieved close to the zero phonon line of the nitrogen-vacancy center with superior emission directivity and collection efficiency. The results have implications in on-demand single photon generation, spin-photon interface, many-body interactions, and strong coupling.

1. Introduction

Wave-scattering is a ubiquitous process not limited to light-matter interactions but applicable to condensed matter systems, nuclear physics, and atmospheric sciences. The measure of wave scattering is quantified using the scattering cross-section, which defines the interaction strength between the incoming particle and scatterers. Optimizing scattering cross-section is a sought-after goal in atomic spectroscopy, nuclear scattering, and light-matter interactions. Specifically, the reliable control over light scattering results in photonic band gap, random lasing, wavefront shaping, and metamaterials that induce an exploration in fundamental science and applications. The scattering optimization plays a pivotal role in modulating the emission dynamics of quantum emitters and spin-photon entanglement using a pre-designed spatial arrangement of sub-wavelength scatterers.

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The generation of on-demand single photons using solid-state emitters has refined the research into spontaneous emission control using photonic metamaterials. The recent surge disseminates that the negatively charged nitrogen-vacancy (NV−) center in a diamond is a room-temperature single photon source with high quantum efficiency and spin coherence time. The NV− center is formed by a substitutional nitrogen atom adjacent to a carbon vacancy in a diamond which finds applications in quantum sensing, magnetometry, and biomarkers. The emission spectrum of NV− center consists of a pure electronic transition (zero phonon line (ZPL)) at 640 nm assisted with broad phonon sideband (PSB) emission. Such PSB transitions induce decoherence with limited 3% emission at ZPL even at low temperatures. However, it is necessary to enhance emission intensity and the rate at the ZPL with simultaneous PSB inhibition for efficient use of NV− center in single photon generation, optical spin readout, and quantum sensing. The reliable control over the emission requires the deterministic tuning of local density of optical states (LDOS). This demands scattering optimization using photonic metamaterials consisting of scatterers with different shapes, geometry, or their compositions. This has realized unique phenomena in atomic antennas meta-materials and light emission. The scattering optimization excites different types of electric and magnetic dipole moments that induce directional light scattering with suppression in either forward or backward scattering. The complete suppression of backward scattering is known as the Kerker condition that occurs as a result of interference between the electric dipole (ED) and magnetic dipole (MD). The role of higher-order modes is studied and the overlapping of electric quadrupole (EQ) and magnetic quadrupole (MQ) modes are discussed to exhibit Kerker condition. The Kerker condition is generalized to different domains that include controlled atomic transitions, Huygens sources, spin-orbit interactions, and invisibility. The dielectric metasurface with directional scattering can significantly modify the quantum emitter properties through LDOS tuning. Hence we anticipate the ZPL enhancement using Kerker condition; a long-awaited goal in NV center-based quantum technology.

In this article, we discuss the emission rate enhancement of a single NV− center at the ZPL wavelength of 640 nm exploiting the Kerker condition in a dielectric metasurface. The constructive interference of several multipoles is evoked to obtain the...
Kerker condition, which is discussed using simulations supported by analytical calculations. The strong field confinement along with unidirectional scattering enables the tuning of the emission rate. An enhancement of 400 times in the emission rate is achieved with strong emission directivity and collection efficiency.

2. Results and Discussions

2.1. The Kerker Condition

Figure 1a shows 2D Silicon (Si) nano-disk arrays to achieve Kerker condition at 640 nm using finite-difference time-domain (FDTD) simulations (Lumerical). The simulations are performed using a plane-wave incident normally on the top of the metasurface (in the −z direction). The optimized parameters of lattice constant (a) 310 nm, diameter (d) 230 nm, and thickness (t) 115 nm on a glass substrate of index 1.5 are used to obtain the Kerker condition. The wavelength (λ)-dependent complex refractive index of Si is taken from the Palik handbook.[22] 

\n
\[ n_0(\lambda) + i\beta(\lambda) \]

where \( n_0(\lambda) \) and \( \beta(\lambda) \) are real and imaginary part of index, and thus losses associated with Si is included in the calculations. An x-polarized plane wave with wave vector \( k \) in the −z direction induces electric and magnetic multipolar resonances decomposed using multipole expansion.[23] Figure 1b depicts a schematic of dipolar resonance consisting of ED and MD originated due to induced polarization. The oscillating ED with dipole moment \( \mathbf{P} \) creates a current loop with density \( j \), which drives the displacement current loop with MD moment \( \mathbf{M} \). The circulating current loop \( j \) in the axial direction constitutes poloidal currents with toroidal dipole moment \( \mathbf{T} \). These dipolar terms can interfere in constructive or destructive ways, under specific conditions, to achieve Kerker condition as shown in Figure 1b.

Figure 2a shows simulated far-field transmission (reflection) spectra from an array of Si nano-disks that exhibit a peak (trough) at 640 nm. This peak originates due to interference between excited multipoles within nano-disk and their interaction with adjacent nano-disks.[24,25] The spectra show 12% reflectivity with 46% transmittance, which illustrates a reduced backward scattering at 640 nm, as expected at Kerker condition. However, 42% of light is absorbed by the Si nano-disks that inhibit a complete forward scattering. A full transparency window with 100% light transmission at 640 nm is obtained for metasurface made with lossless material (β = 0) with λ-dependent \( n_0 \) value, as seen in the inset of Figure 2a. Our results substantiate that null backward scattering is restricted by finite absorption (Section SI, Supporting Information). The simulation results are corroborated with analytical calculations using the multipole expansion method (Section SI, Supporting Information).

We estimate cartesian multipoles contributing to the total scattering cross-section \( C_{\text{scat}} \) using FDTD simulations and the multipole expansion method.[30] A plane wave incident normally in the −z direction excites the resonances associated with metasurface. The electric field and refractive index profile values at each grid point of the x–y–z directions are obtained using FDTD simulations. Then, the frequency (f) dependent x–y–z components of the electric field \( \mathbf{E}(x,y,z,f) \) and refractive index \( n(x,y,z,f) \) are extracted from the simulations and imported to MATLAB script to calculate the decomposed multipoles and \( C_{\text{scat}} \). The induced displacement current density is:

\[ j(t) = -i\omega\varepsilon_0\varepsilon - i\omega\mathbf{E}(t), \]

where \( \mathbf{E}(t) \) is the field at position vector \( r \), \( \omega = 2\pi f \) is the angular frequency, \( \varepsilon \) and \( \varepsilon_0 \) are the permittivity of metasurface and free space with \( \varepsilon_0 = 1 \) as a homogenous medium. The Kerker condition arises due to the interference between the ED and MD with dipole moments \( \mathbf{P} \) and \( \mathbf{M} \), given by:

\[ \mathbf{P}_\alpha = -\frac{1}{i\omega} \int j_\alpha d^3r \quad \text{and} \quad \mathbf{M}_\alpha = \frac{1}{2} \int \mathbf{r} \times j_\alpha d^3r \quad \text{with} \quad \alpha = (x,y,z). \]

The poloidal current generates TD contribution in the scattering spectra given by \( \mathbf{T}_\alpha = \frac{1}{10\omega c} \int [(\mathbf{r} \times j) r - 2r^2 j_\alpha] d^3r \).

The higher order multipoles such as EQ and MQ also contribute to scattering, expressed as:

\[ \mathbf{EQ}_{\alpha\beta} = -\frac{1}{10\omega} \int \left[ \frac{4}{5} r_\alpha r_\beta (r \cdot j) - 2(r \cdot j) \delta_{\alpha\beta} \right] d^3r \]

\[ + k^2 \int \left[ 4r_\alpha r_\beta (r \cdot j) - 5r^2 (r_\alpha j_\beta + r_\beta j_\alpha) + 2(r^2 (r \cdot j) \delta_{\alpha\beta}) \right] d^3r \]

\[ \mathbf{MQ}_{\alpha\beta} = \frac{1}{10\omega} \int \left[ r_\alpha (r \times j) + r_\beta (r \times j) \right] d^3r \]

where \( \delta_{\alpha\beta} \) is Kronecker delta function with \( \delta_{\alpha\beta} = 1 \) for \( \alpha = \beta \) and \( \delta_{\alpha\beta} = 0 \) otherwise, with \( \alpha, \beta = x, y, z \), and \( k = \omega / c \) where \( c \) is the speed of light in vacuum. The scattered field is sum of the contribution from all multipoles to \( C_{\text{scat}} \) given as:

![Figure 1](https://example.com/f1.png)

**Figure 1.** a) Schematic of metasurface consists of a square array of Si nano-disks with \( d = 230 \) nm, \( t = 115 \) nm, and \( a = 310 \) nm on glass with an incident x-polarized plane wave in the −z direction. b) The constructive interference between the electric (P), magnetic (M), and toroidal (T) dipole moments P, M, and T results in complete forward scattering with null backward scattering.
C_{\text{scat}} = \text{ED} + \text{TD} + \text{MD} + \text{EQ} + \text{MQ}, \text{ which after substitution gives:}^{[23]}

\begin{align*}
C_{\text{scat}} &= \frac{k^4}{6\pi^2 \varepsilon_0} |\mathbf{P}_\alpha|^2 + (ik)^2 |\mathbf{T}_\alpha|^2 + \left| \mathbf{M}_\alpha \right|^2 + \frac{1}{120} k^2 |\mathbf{FQ}_{\alpha}|^2 \\
&+ \frac{1}{120} \left| \mathbf{MQ}_{\alpha} \right|^2 \tag{3}
\end{align*}

The observed transmission peak at 640 nm in Figure 2a corresponds to enhanced forward scattering arising due to multipole interference. Hence, it is necessary to calculate the multipolar contributions to the spectral-dependent C_{\text{scat}} using Equation (3).^{[26]} Figure 2b shows the superposition (solid line) of scattered fields arising from different types of excited multipoles. The calculated C_{\text{scat}} is peaked at 640 nm, similar to the transmission peak. Conventionally, Kerker condition is explored as an overlap of ED and MD only, neglecting the higher-order terms.\(^{[27]}\) However, we have observed that TD (dotted line), ED (dashed line), and MQ (dash-dot-dash line) moments are the dominant multipoles contributing to C_{\text{scat}} at 640 nm, as seen in Figure 2b. The contribution from MD (line with circles) and EQ (line with squares) is quite minimal. Hence, our results correspond to the generalized Kerker effect originated due to the contributions from TD, ED, and MQ modes. The ED and TD scattered fields are analyzed using their phases and amplitudes (Section SII, Supporting Information). The nearly same phase confirms the constructive interference between the ED and TD creating a super-dipole effect, which collectively constitutes a total electric dipole (TED). This is in contrast to an anapole-like mode where a destructive interference between ED and TD is observed.\(^{[28]}\) Similarly, the TED and MQ modes constructively interfere with each other, while a destructive interference between the TED and MD modes is seen in the scattering spectra that inhibit forward scattering. Figure 2c shows the normalized electric field intensity distribution \(\frac{|E|^2}{|E_0|^2}\), where \(|E|^2\) is field intensity at 640 nm in comparison to the incident field intensity \(|E_0|^2\). The arrows indicate the vector distribution of the induced displacement current. The cross-sectional (x–z plane) view shows an enhanced intensity by a factor of 15 at nano-disk center and then reduces to the edges. Such a field enhancement is obtained due to constructive interference of several multipoles with optimized scattering that can impart significant modification to the emission rate of single NV\(^-\) center.

2.2. Emission Enhancement

The spontaneous emission rate of a dipole emitter with transition dipole moment \(\mathbf{d}\) depends on the environment through LDOS.\(^{[29]}\) The strong optical field induced by the excitation of electric and magnetic multipoles is related to LDOS \(\rho_{\alpha}\) that measures the emission decay rate \(\Gamma\) at a position \(r_0\) as 

\[\Gamma = \frac{\pi \omega_0 |\mathbf{d}|^2}{\hbar} \rho_{\alpha}(r_0, \omega_0).\]

Here \(\rho_{\alpha}(r_0, \omega_0) = \frac{2\omega_0}{\pi\varepsilon_0 c} |n \cdot \text{Im}(G(r, r_0, \omega_0))| n\) and \(G(r, r_0, \omega_0)\) is Dyadic Green’s function which represents the electric field at \(r\) due to a dipole at \(r_0\).\(^{[30,31]}\) A significant electric field enhancement upon a plane-wave excitation is observed at the Kerker condition of 640 nm in Figure 2c and hence, the metasurface acts as an optical cavity at Kerker condition. This anticipates for an increased LDOS at 640 nm (corresponds to \(\omega_0\)) that should result in large decay rate enhancement. It is quite often reported that emission intensity enhancement is taken as a measure of dipole excitation in metasurfaces.\(^{[32]}\) However, emission intensity enhancement is a convoluted result of several parameters including the excitation pump intensity, variation in photonic environment, enhanced detection efficiency, and quenching effect. Hence, variation in intensity is an insufficient criterion to claim that LDOS is enhanced due to Kerker condition. Thus, emission rate calculation is necessary to ascertain emission enhancement due to Kerker condition.

We have calculated the wavelength-dependent relative LDOS (symbols) for a single emitter (single NV\(^-\) center in a nanodiamond of radius 20 nm and index 2.45) placed at each nano-disks center \((x = 0, z = 0\) in Figure 2c). The relative LDOS implies the ratio between the calculated LDOS for the emitter embedded within each nano-disks to the calculated LDOS for the emitter placed in vacuum. This single emitter acts as a point dipole source with emission spectral range of 550–750 nm. Figure 3a shows that the calculated wavelength-dependent relative decay rate (line) exhibits a significant increase at 640 nm, following the relative LDOS enhancement at the Kerker condition. The relative decay rate is defined as the decay rate of the emitter embedded in each nano-disks of metasurface having a decay rate \(\Gamma_0\) to the decay rate \(\Gamma_0\) of the emitter placed in vacuum. The relative decay rate and relative LDOS conclude the same results as expected for an emitter with near-unity quantum efficiency like NV\(^-\) centers in nanodiamond. A slight shift in the wavelength is due to reflections at the boundaries of the
finite size of the computational domain. Since, in experimental studies, the relative decay rate is often measured to support the LDOS changes, hence we have shown the relative decay rate changes also in Figure 3a. The estimated rate enhancement ($\Gamma/\Gamma_0$) of 400 times with narrow emission bandwidth of 40 nm at room temperature is achieved due to spectral overlap between ZPL and Kerker condition at 640 nm. The increase in $\rho_0$ is due to the constructive interference between the TED and MQ which enhances the emission rate of NV$^-$ ZPL using the Kerker condition. An emission rate enhancement of 180 times is also obtained for an emitter positioned at the top surface of each nano-disk ($z = 0$ nm; $z = 575$ nm).

Figure 3a inset shows the spatial-dependent variation of $[E(n_0)]^2$ (symbols) at 640 nm for an emitter located at different z-values within each nano-disk for $z = 0$ nm. Here, the field intensity variation is obtained by the excited multipoles induced by the embedded emitter within the nano-disks. We have obtained an electric field intensity enhancement due to the constructive interference between the TED and MQ which enhances the emission rate of NV$^-$ ZPL using the Kerker condition. An emission rate enhancement of 180 times is also obtained for an emitter positioned at the top surface of each nano-disk ($x = 0$ nm; $z = 575$ nm).

2.3. Emission Directivity

In addition to emission rate enhancement, emission directivity from a single emitter maneuvered by the excited multipoles is an important factor to be considered. Figure 4 shows the calculated 2D angle-dependent far-field emission radiation pattern from the single emitter coupled to the metasurface in the $x$–$z$ plane. The 2D radiation pattern ($S(\theta, \varphi)$) is calculated using the angular distribution of emitted power $P(\theta, \varphi, \lambda_\nu)$ as:

$$S(\theta, \varphi) = \frac{P(\theta, \varphi, \lambda_\nu)}{\max \{ P_\nu(\theta, \varphi, \lambda_\nu) \}} |E|_0^2$$

(4)

where $P_\nu(\theta, \varphi, \lambda_\nu)$ is the emitted power in a vacuum at the emission wavelength $\lambda_\nu$, $\theta$, $\varphi$ are the polar and azimuthal angles.
respective. The directional nature of emission results from the constructive interference between the emitter and excited multipoles. The plane-wave excitation is expected to result in an angular distribution mainly restricted to the forward scattering direction of the propagating plane wave at Kerker condition. The angular distribution observed in general is quite broad and extends over the whole forward hemisphere.[21–36] Figure 4a shows the angular distribution of the normalized radiation intensity for horizontal in-plane dipole, as the single emitter, placed on top of a glass substrate (red line) and in a vacuum (green line) at 640 nm. The emitter does not consider forward or backward scattering and emits evenly in all directions. The emitted radiation from an emitter placed on the substrate is asymmetric in z-direction due to the high-index glass substrate at the bottom and air on the top.

Figure 4b shows the asymmetric radiation pattern along the z direction for the emitter placed at the nano-disk center. The radiation lobe in the lower half (180° < θ < 360°) is restricted to smaller angular range in comparison to the upper half (0° < θ < 180°). Since, the spontaneous emission from a radiating emitter is independent of the excitation process, both vertical directions (top and bottom) are expected to be symmetric. However, the observed asymmetry in radiation pattern arises due to the presence of the glass substrate and air. We notice an enhancement of ∼300 times in the far-field radiation intensity (normalized to maximum vacuum intensity) at 640 nm (red line). However, the enhancement is obtained only perpendicular to the emitter axis (parallel to x-axis) within a limited angular range. This indicates that the emission pattern direction is induced by the constructive interference between emitted field from the emitter and the scattered field by the TED and MQ. The radiation pattern is symmetric with z-axis due to the even parity of TED and MQ modes.[16] The radiation pattern at an off-resonance wavelength of 540 and 740 nm shows relatively low enhancement by a factor of two and eight times in contrast to 640 nm (Section SIII, Supporting Information).

The directional emission can be further enhanced with a reduced angular range using a reflector layer beneath the metasurface. The silver layer with a thickness of 100 nm acts as a reflector that enhances the radiation intensity to a value of more than 6 × 10^4 in the reflection geometry as shown in Figure 4c. Further, the collection efficiency (η) is calculated as $I_{\text{collection}}/I_{\text{total}}$ with $I_{\text{collection}}$ as the radiated emission intensity in the presence of metasurface and $I_{\text{total}}$ as the radiated intensity over a 360° solid angle. The calculated collection efficiency is 70% at 640 nm using a collection objective of numerical aperture 0.9 (solid angle: 64.15°) without the reflector layer from the metasurface. The efficient coupling to a single-mode fiber could be substantially improved by considering metasurface on top of the reflector layer with very large emission directionality with near-unity collection efficiency of 99.9% using similar collection geometry. The proposed metasurface at Kerker condition provides better collection efficiency, directivity, and emission enhancement for a single NV+ center.

Since the quantum emitter’s radiation pattern corresponds to a radiating point dipole, it is reported that the emission exhibits weak directionality and low collection efficiency.[37] Our studies demonstrate that quantum emitter integrated with metasurfaces provide high directionality while improving its collection efficiency using Kerker condition. The observed modification in emission rate is not limited to single NV centers in diamond, rather it can be generalized to a variety of emitters in SiC and h-BN.[38,39] The present system can be realized using stacked material growth composed of Si/SiO$_2$(embedded with nanodiamond)/Si, and the structure is further etched to create the 2D array of Si nano-disks containing NV+ center. A similar kind of fabrication process is discussed for embedding Er$^{3+}$ ions in Si nanoslots.[40] Further, the work can be extended to structures made using other materials, for example, SiC based metasurface. In such SiC based structures, creating defects centers like vacancy of Si, C, or di-vacancy is quite possible by ion irradiation. The Kerker mode switching can be achieved by a rapid change in the refractive index through the optical Kerr effect or free carrier generation.[41] Such Kerker-based optical switching, combined with single NV+, enables deterministic generation of single photon source or through the timing of the pump excitation to the metasurface. Further, with the incorporation of excitonic materials, the strong coupling for excitons can be achieved using Kerker condition.[42] The Kerker condition is tunable through the appropriate choice of lattice constants and materials so that it can be achieved at any frequency. This is useful for the better readout of NV$^+$ spins with enhanced sensitivity and high-fidelity utilizing the Kerker condition tuned at microwave frequency. Such Kerker-based spin readout can be an alternative approach to the conventional micro-wave cavity-based approach.[43] Thus, our results encompass broad domains of interest and are applicable to any kind of wave-wave scattering in an appropriate medium.
3. Conclusions

To conclude, we have studied Kerker condition induced enhancement in the emission rate of a single NV center close to the ZPL wavelength of 640 nm. A complete forward scattering is obtained at the Kerker condition using simulations supported by analytical calculations. The Kerker condition is originated due to the constructive interference between ED and TD, which forms a super-dipole effect combined with the contribution from MQ. Further, decay rate enhancement of 400 times is obtained at Kerker condition with a strong directivity and collection efficiency. The emission rate enhancement depends on the emitter position within nano-disk vis-à-vis the localized field intensity with maximum rate enhancement at the nano-disk center. Our results substantially reinforce the research in quantum metasurfaces by exploiting the Kerker condition for generating on-demand single photon source, quantum imaging, many-body interactions, and strong coupling between emitters.

Supporting Information

Supporting Information is available from the Wiley Online Library or from the author.

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Conflict of Interest

The authors declare no conflict of interest.

Data Availability Statement

The data that support the findings of this study are available from the corresponding author upon reasonable request.

Keywords

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