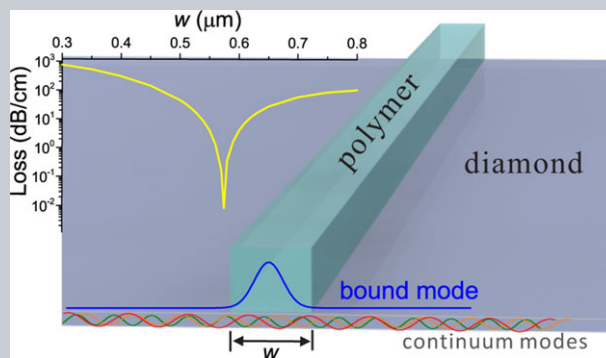


Abstract Light is usually confined in photonic structures with a band gap or relatively high refractive index for broad scientific and technical applications. Here, a light confinement mechanism is proposed based on the photonic bound state in the continuum (BIC). In a low-refractive-index waveguide on a high-refractive-index thin membrane, optical dissipation is forbidden because of the destructive interference of various leakage channels. The BIC-based low-mode-area waveguide and high- Q microresonator can be used to enhance light–matter interaction for laser, nonlinear optical and quantum optical applications. For example, a polymer structure on a diamond membrane shows excellent optical performance that can be achieved with large fabrication tolerance. It can induce strong coupling between photons and the nitrogen–vacancy center in diamond for scalable quantum information processors and networks.



Guiding light through optical bound states in the continuum for ultrahigh- Q microresonators

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1. Introduction

Great progress has been achieved recently in photonic integrated circuits (PICs) for classical and quantum information processes [1, 2]. Efforts have been made to exploit new materials, such as materials with excellent nonlinear optical properties [3–6] and solid quantum emitters [7, 8], for better optical performances and functionality. Meanwhile, a range of new physical phenomena has also been studied in PICs and applied to develop new components, including the photonic Aharonov–Bohm effect [9] and topological insulators [10, 11]. In PICs, photons are processed by basic components composed of waveguide and resonator structures, where a high refractive index contrast to the environment is essential. It has long been known that the light in a low-refractive-index structure will leak through coupling to continuum modes in the substrate. This can be intuitively explained by quantum physics in that the wave cannot be localized upon a potential well. Thus, the materials for PICs are restricted to those of high refractive index. However, fabrication difficulties are often encountered for some high-refractive-index materials, such as diamond, whose optical performances suffer from the surface scattering caused by sidewall roughness [12, 13].

It is instructive to consider low-refractive-index PICs. Actually, bound states do exist above a potential barrier. This intriguing phenomenon, the so-called bound state in

the continuum (BIC), was first proved by von Neumann and Wigner in 1929 [14], and has been extensively studied recently in electronic and photonic structures [15–21]. In this paper, we study the mechanism of BIC and propose a novel photonic BIC-based waveguide, which is made of a low-refractive-index material on a high-refractive-index substrate, without specially engineered potential distribution [18] or multiple waveguides by virtue of symmetry [19]. In such a hybrid waveguide, optical dissipation is forbidden because of the destructive interference of various dissipation channels under certain geometric parameters. Remarkably, such BIC-based guided modes can also be used in rotating-symmetry microring structures to allow ultrahigh quality factor resonances. Therefore, our study brings the BIC from the basic scientific interest of fundamental quantum physics to practical applications, permitting a new kind of PIC. In this work, we take diamond as an example, for the reason that photonic structure is very necessary to enhance the emission and collection of the zero-phonon line (ZPL) of the nitrogen–vacancy (NV) center in diamond, then to improve the fidelity in quantum control [22, 23] and the resolution in magnetic and biologic sensing [24, 25] with the NV center. By combining the NV centers and fabrication-friendly polymer photonic structures on a diamond membrane, strong light–matter interaction is promising. The BIC-based diamond chip provides an excellent platform for integrated quantum networks [26].

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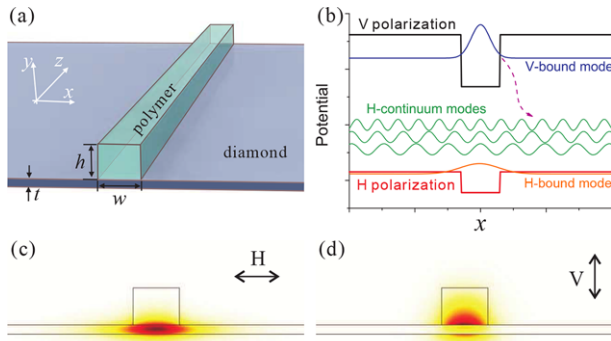


Figure 1 Low-refractive-index structure on high-refractive-index substrate. (a) The hybrid photonic BIC structure with a polymer waveguide on a thin diamond membrane. (b) The effective potential for modes. (c, d) Field distributions of horizontal (H) or vertical (V) polarized modes bound to the waveguide, with polymer waveguide height $h = 400$ nm and width $w = 500$ nm, and membrane thickness $t = 100$ nm.

2. Limitation of refractive index

The light propagating in a waveguide along the z -axis with slowly varying approximation can be described by

$$-i2\beta\partial_z\psi(\mathbf{r}) = [\nabla^2 - U(\mathbf{r})]\psi(\mathbf{r}). \quad (1)$$

Here, the potential is $U(\mathbf{r}) = \beta^2 - n^2(\mathbf{r})k^2$, where $n(\mathbf{r})$ is the dielectric refractive index and $k = 2\pi/\lambda$ is the vacuum wavenumber. $\psi(\mathbf{r})e^{i\beta z - i\omega t}$ is the scalar wave function, and ω and β are the light frequency and propagation constant, respectively. The equation is analogous to the Schrödinger equation, with time-dependent evolution replaced by the spatial-dependent (z) evolution. It is well known in quantum mechanics that a particle can be confined in a finite potential well, while the probability to find it outside the well exponentially decays and leads to quantum tunneling. As a consequence, a waveguide made of high-refractive-index material can support bound modes, which satisfy $U(\mathbf{r}) > 0$ outside the potential well, and the evanescent field of bound modes outside the waveguide enables interaction between waveguides through tunneling. However, in the case of a waveguide with refractive index lower than the environment, the potential well becomes a potential barrier in some ways, and then bound modes couple to continuum modes in the environment and lead to significant leaking loss.

To construct PICs beyond the limitation of refractive index, we consider a hybrid structure consisting of a polymer waveguide (refractive index $n_p = 1.49$) on an air-suspended diamond membrane ($n_d = 2.41$) as depicted in Fig. 1a. In this film-like substrate, wave functions are confined along the y -direction, and the engineered continuum is reduced to one dimension (along the x -axis). Under the two-dimensional approximation by treating the regions with

and without polymer both as film waveguides separately, the Schrödinger equation is reduced to [27]

$$-i2\beta\partial_z\psi(x, z) = [\partial_x^2 - U(x)]\psi(x, z). \quad (2)$$

Here, $n(x)$ in $U(x)$ is replaced by the effective one-dimensional refractive index. In the following, we focus on the working wavelength $\lambda = 637$ nm (ZPL of NV centers). The effective refractive indices of the fundamental propagating mode of the film waveguide are calculated as $n_{1,H(V)} = 1.879$ (1.536) and $n_{2,H(V)} = 1.820$ (1.171) for regions with and without polymer for horizontal (vertical) polarization, respectively.

As shown in Fig. 1b, the polymer waveguide induces a potential well which gives rise to bound modes. Figures 1c and 1d show two fundamental bound modes with different polarizations, which are obtained by solving Maxwell equations numerically without one-dimensional approximations [28]. Since the depth of the potential well for the horizontal-polarized bound mode (HBM) is much lower than that for the vertical-polarized bound mode (VBM), the HBM is weakly confined in the membrane and widely distributed along the x -direction, while the VBM is strongly confined laterally. This result suggests very large loss of HBM for bending waveguides in practical applications. Therefore, we restrict the study to VBM in the following.

3. Coupling strength

It is intuitively obvious that the VBM can dissipate through coupling to infinite horizontal-polarized continuum modes (HCMs) above the potential barrier, since the energy of the VBM is much higher than the potential barrier of HCMs (Fig. 1b). The Hamiltonian for the VBM coupling with continuum modes can be written as ($\hbar c = 1$)

$$H = \beta_b b^\dagger b + \sum_m \beta_m c_m^\dagger c_m + \sum_m (g_m c_m^\dagger b + \text{h.c.}). \quad (3)$$

Here integer m is the order of HCM, b and c_m are respectively annihilation operators of the VBM and m th HCM, β_b and β_m are the corresponding propagation constants and g_m is the coupling strength between the VBM and m th HCM.

In order to solve the coupling strength between the waveguide bound mode and the continuum modes, we firstly study numerically the case of a finite slab of width s [28]. In this case, HCMs are discrete as horizontal-polarized slab modes (HSMs) under the quantization condition $k_x s \approx 2\pi m$. Here, the wave vector along the x -direction is $k_x = \sqrt{n_{2,H}^2 - n_m^2}k$, with the effective mode index $n_m = \beta_m/k$. Figure 2a shows the numerically solved effective mode indices of eigenmodes in the hybrid waveguide [28], where $n_m \approx \sqrt{n_{2,H}^2 - (2\pi m/ks)^2}$ changes with s while the effective mode index of the VBM $n_b = \beta_b/k$ is constant. When the VBM and HSMs are near resonance ($n_m \approx n_b$), there are two different behaviors in the trajectories of the mode index against s : crossing when m is odd

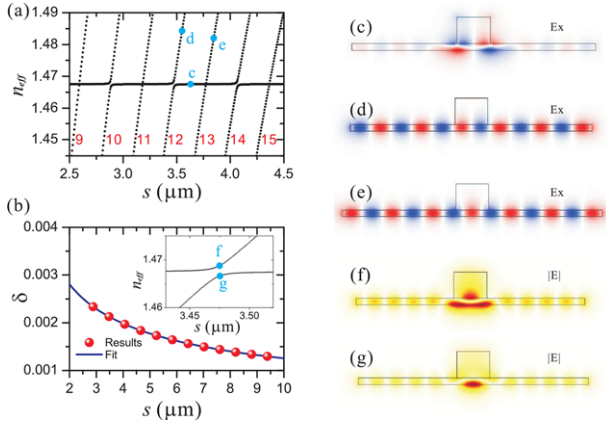


Figure 2 Calculation of coupling strength. (a) The effective mode indices of VBM and HSMs with varying slab width s . (b) The minimal effective mode index differences at anti-crossing. Inset: anti-crossing for $m = 12$. (c–g) Field distributions of s denoted in (a) and (b), with the same h , w and t as in Fig. 1.

and anti-crossing when m is even. To interpret these results, the profiles of the horizontal component of electric field (E_x) for VBM and HSMs are plotted in Figs. 2c–e [28]. Although the electric field of VBM is vertically polarized, its E_x is nonzero at corners due to diffraction (Fig. 2c). The parity of E_x of the VBM is odd while the parity of the m th HSM is determined by m (Figs. 2d and e). When m is odd, the VBM is orthogonal with the m th HSM and their mode index trajectories cross each other without interplay. However, for even m , the overlap between wave functions of VBM (φ_b) and m th HSM (φ_m) will induce coupling.

Due to the interaction, the eigenmodes of this hybrid waveguide are a hybridization of VBM and HSMs, showing an effective index difference between the new eigenmodes as $\delta = \sqrt{4g_m^2 + \Delta^2}/k$, with $\Delta = (n_m - n_b)k$. This means that it is nonzero g_m that leads to the anti-crossing because δ is always greater than zero. As an example, a detailed illustration of anti-crossing between the VBM and 12th HSM is shown in the inset of Fig. 2b. When the two modes are on-resonance ($n_{12} = n_b$), the splitting between two eigenmode branches reaches the minimum ($\delta = 2g_{12}/k$), with hybrid eigenmodes shown in Figs. 2f and 2g. The coupling strength g_m depends on the normalized field overlap between VBM and HSM, which is approximately proportional to $1/w\sqrt{s}$. As shown in Fig. 2b, the minimums $\delta = 2g_m/k$ which are deduced from Fig. 2a are plotted and are consistent with the curve fitted by $1/\sqrt{s}$.

4. BIC in hybrid waveguide

There are two channels for the VBM to dissipate to each continuum mode due to scattering at corners of the waveguide. As shown in Fig. 3c, the energy of the VBM is embedded in the continuum spectrum of the left-going ($-x$)

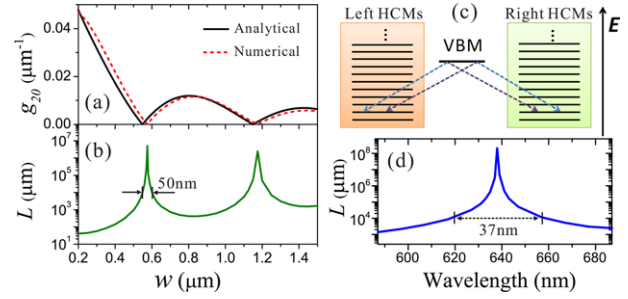


Figure 3 BIC in hybrid waveguide. (a) The coupling strength g_{20} against waveguide width w . The solid line is the analytical result, and the dashed line is the numerical simulation result. (b) The propagation length of the bound waveguide modes for $s = \infty$ against the waveguide width with $\lambda = 637$ nm. (c) A schematic illustration of the BIC for the VBM coupled to the HCMs. (d) The calculated propagation length L of VBM for $s = \infty$ against wavelength, with $w = 575$ nm.

and right-going (x) HCMs. As a consequence, the effective coupling strength of VBM with m th HCM is

$$g_m \approx \tilde{g}_m \times \frac{|1 + e^{ik_x w}|}{2w\sqrt{s}}, \quad (4)$$

which contains the interference of two channels with phase difference $k_x w \approx \sqrt{n_{2,H}^2 - n_m^2}kw$, where s is the width of substrate and $\tilde{g}_m$ is a constant which can be solved by numerical simulation. Equation (4) illustrates the essential physical principle of BIC for eliminating the losses to the continuum: constructing multiple loss channels and controlling the phase differences between them to realize destructive interference. This principle can also be generalized to many other systems that couple to one-dimensional or two-dimensional continuum.

For an infinitely wide substrate, the bound state coupling to infinite continuum modes leads to Markov system–environment interaction [29], and thus the energy of the VBM decays exponentially with propagation as $I(z) = I(0)e^{-z/L}$. For the density of continuum modes

$$\rho \approx \frac{n_b}{\sqrt{n_{2,H}^2 - n_b^2}} \times s, \quad (5)$$

the decay length of the bound mode is

$$L = \frac{1}{2g_m^2 \rho}. \quad (6)$$

Noting that the mode density is proportional to s , while g_m is proportional to $1/\sqrt{s}$ (Eq. (4)), then we have

$$L \approx \frac{w^2}{\tilde{g}_m^2 \cos^2(k_x w/2)} \frac{\sqrt{n_{2,H}^2 - n_b^2}}{2n_b} \quad (7)$$

is independent of s . Therefore, the properties of BIC for infinite s can be obtained by solving the coupling strengths

and mode density of finite s . Equation (7) indicates that the dissipation of the VBM can be totally frozen ($L \rightarrow \infty$) by carefully choosing the geometry of the polymer waveguide: when $\cos(k_x w/2) = 0$ is achieved, the dissipation is forbidden because of destructive interference, leading to a photonic BIC.

To confirm this conclusion, we calculate g_{20} as a function of w numerically. For each waveguide size, g_{20} are obtained by calculating the anti-crossing of the bound mode and 20th HSM, as shown in the inset of Fig. 2b. As shown in Fig. 3a, the numerical data of g_{20} agree well with Eq. (4), showing oscillations and approaching zero for certain w . Based on the numerically evaluated coupling strengths and mode density, the dependence of L on w and λ is calculated according to Eq. (6), as plotted in Figs. 3b and 3d. The decay length is increased dramatically for certain parameters, corresponding to the BIC where the VBM is almost totally decoupled from the continuum modes. These results indicate that L can be larger than 1 m for the low-refractive-index waveguide on high-refractive-index substrate.

5. Ultrahigh- Q hybrid microresonator

A microresonator is another important component in a PIC, which can trap light and enhance the light–matter interaction. Figure 4a shows a typical microring resonator, whose geometry is characterized by the width of the cross section (w_r) and exterior radius (R). For the vertical-polarized whispering gallery modes (WGMs), similar to the waveguide VBM, the bound modes will inevitably couple to the continuum modes, which will induce extra energy loss and limit the Q -factor of the WGMs. In such an axis-symmetry structure, the WGMs couple to the horizontal-polarized cylindrical waves in membrane $J_q(nkr)e^{iq\phi}$, where $J_q(z)$ is the q -th order Bessel function [30]. Since the mode profile of WGMs tends to the outer corner (Fig. 4b), the two passages of dissipation (scattering at two corners) are unbalanced. Therefore, the cylindrical system is significantly different from the one-dimensional waveguide. Here, the eigenmodes of the microring resonator are solved numerically using an effective two-dimensional axisymmetric model [28, 31, 32].

To test whether the losses to the continuum can be forbidden, as in the waveguide BIC, in such cylindrical symmetric photonic structures, the loss of the bound mode to the continuum is estimated from $|J_q(nkR) - \xi J_q(nk(R - w_r))|$ (Fig. 4d). Here, the two terms correspond to the loss channels of interior and exterior corners, which are proportional to the electric field overlap at the corners. The factor $\xi < 1$ accounts for the ratio of electric field of bound mode at interior and exterior corners. The loss shows oscillation and its minimum can reach zero, which is due to the quasi-standing-wave behavior of cylindrical Bessel wave in the radius direction. The prediction of the cancellation of losses to the continuum is confirmed by the numerical calculation of Q of WGMs against R with wavelength around 637 nm (Fig. 4e). There are several peaks of the Q -factor, indicating

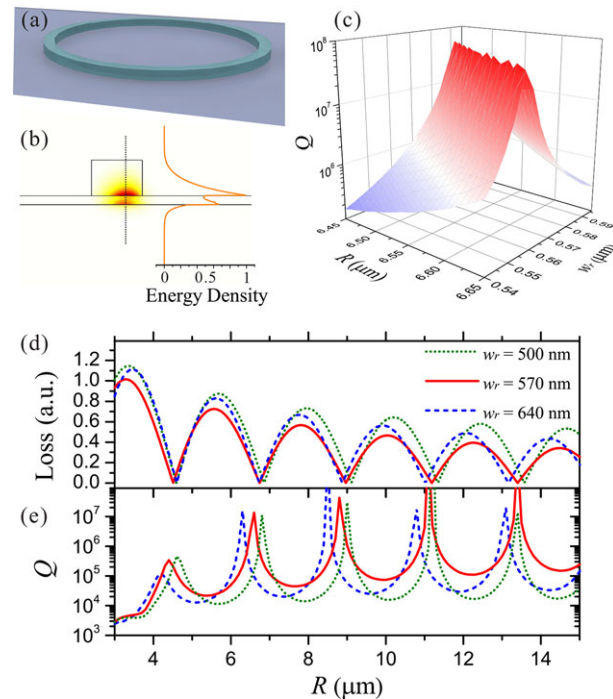


Figure 4 BIC in a cylindrical symmetric structure. (a) A schematic of the hybrid microring. (b) The energy density distribution at the cross section of the hybrid microring. The solid curve is the field distribution along the y -direction, as indicated by the dashed line. (c) The tolerance of the Q -factor versus R and microring width w_r . (d) Predicted loss and (e) calculated Q -factor of the microring against the radius R , with various microring widths.

the dissipation channels to the substrate are canceled out for specific R . The peak values of the Q -factor are only limited by the inevitable bending radiation loss, which grows exponentially with the ring radius. It is worth noting that horizontal-polarized WGMs are not found in our numerical simulations, due to their extremely low Q -factor caused by very large bending loss of HBM.

6. Strong coupling

Benefiting from the Purcell effect [33], the coherent ZPL emission of NV centers embedded in diamond will be enhanced by interacting with bound photonic modes. Extensive efforts have been made to achieve high Purcell factors [12, 13].

For the BIC in the waveguide, the enhanced spontaneous emission to the bound waveguide mode is determined by the Purcell factor $F = \frac{3}{4\pi} \frac{\lambda^2}{A} \frac{c}{v_g}$, where A is the effective mode area at the cross section of the waveguide, c is the velocity of light in vacuum and v_g is the group velocity of the waveguide mode. For $w = 570$ nm, we have $A = 0.092 \mu\text{m}^2$ and $F = 2.74$, resulting in a waveguide collection efficiency of ZPL $\zeta = F/(F + 1) = 0.73$. In addition to the enhanced emission and collection, the

undesired phonon sideband emission of NV centers can be suppressed as the BIC can only exist around the ZPL (Fig. 3d).

For the microring with $w_r = 0.57 \mu\text{m}$ and $R = 6.6 \mu\text{m}$, the Q -factor of WGMs is as high as 6.5×10^7 for BIC. The mode volume for NV centers in diamond is $V = 1.89 \mu\text{m}^3$, which can be approximated by πRA as the mode profile of WGMs at the cross section is close to that of the waveguide. In such a high Q/V hybrid microresonator, the Purcell factor of the ZPL can be as large as $F = \frac{3}{4\pi^2} \frac{Q}{V} \left(\frac{\lambda}{n_d}\right)^3 = 828$. The maximum coherence coupling strength between photon and zero-phonon transition of NV centers is $G = \sqrt{(\omega d^2/2\hbar\epsilon V) \times \eta} \approx 242 \times 2\pi \text{ MHz}$, where d is the dipole momentum and $\eta = 0.05$ is the percentage of ZPL in the total emission of the NV center. As the decay rate of the NV center is $\gamma \approx 13 \times 2\pi \text{ MHz}$, strong coupling ($G > \gamma, \kappa$) can be achieved when the cavity dissipation rate $\kappa = \omega/2Q < G$, i.e. $Q > 10^6$. For a practical experiment, the dependence of the Q -factor on R and w_r is depicted in Fig. 4c, showing good fabrication tolerance (about 50 nm) of the BIC for strong coupling.

7. Conclusion and outlook

Based on the BIC, the proposed structure is feasible in experimental demonstration. A single-crystal diamond membrane can be prepared by chemical methods [34, 35], and its surface roughness can be reduced to a few nanometers by mechanical polishing or phonon-assisted etching [36]. As for the polymer nanostructures, which possess excellent optical properties and are compatible with other materials [37], they can be fabricated via mature nanofabrication techniques, such as electron beam lithography, nanoimprinting and direct laser writing. In addition, the BIC shows fabrication tolerance of a wide range of parameters. For example, ensuring $L > 10 \text{ nm}$, the fabrication tolerance of w and the wavelength bandwidth are about 50 nm and 37 nm, respectively. It is worth noting that the diamond membrane does not necessarily have to be air-suspended: it can be supported on a low-refractive-index polymer or silica substrate.

Such a photonic BIC structure has shown good optical performance for diamond-based photonic applications and various applications with NV centers. The general principle of BIC can also be extended to other low-refractive-index structures on high-refractive-index substrates. For a photonic BIC-based waveguide with nonlinear optical materials, the optical mode with small mode area can be used to enhance the nonlinear interaction, which is very promising in chip-scale nonlinear optical applications for novel optical phenomena. Lasers can be generated with the simple designed microring structure on an optical gain substrate. The photonic BIC structure also shows potential in the application of new optical materials without complex nanophotonic fabrication.

In addition, the propagation length of the BIC-based waveguide and Q of BIC-based microresonator propor-

tional to $1/\cos^2(kw/2)$ are singular at $\cos^2(kw/2) = 0$, and thus show ultra-sensitivity to the change of structure and wavelength parameters at this singular point. Therefore, BIC provides an alternative way to control the dissipation of photonic devices, and can be applied in optomechanics, sensors and optical switches.

In conclusion, we have proposed and demonstrated photonic BIC in a low-refractive-index waveguide on a high-refractive-index substrate. In addition, photonic BIC also enables ultrahigh- Q microring resonators, which are basic building blocks for the PICs and feasible for experiments. The circuit with polymer on diamond membrane with low-loss BIC has a fabrication tolerance of about 50 nm. Strong coupling between the ZPL transition of NV centers and photons is possible, offering an excellent platform for future scalable quantum information processors and networks. Such a photonic BIC structure will also benefit many chip-scale optical applications in classical and quantum optics.

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