Creation and manipulation of bound states in continuum with lasers: Applications to cold atoms and molecules

Bimalendu Deb¹ and G. S. Agarwal²

¹ Department of Materials Science, Raman Center for Atomic, Molecular and Optical Sciences, Indian Association for the Cultivation of Science, Jadavpur, Kolkata 700032, INDIA.
² Department of Physics, Oklahoma State University, Stillwater, OK 74078, USA.

Abstract

We show theoretically that it is possible to create and manipulate a pair of bound states in continuum in ultracold atoms by two lasers in the presence of a magnetically tunable Feshbach resonance. These bound states are formed due to coherent superposition of two electronically excited molecular bound states and a quasi-bound state in ground-state potential. These superposition states are decoupled from the continuum of two-atom collisional states. Hence, in the absence of other damping processes they are non-decaying. We analyze in detail the physical conditions that can lead to the formation of such states in cold collisions between atoms, and discuss the possible experimental signatures of such states. An extremely narrow and asymmetric shape with a distinct minimum of photoassociative absorption spectrum or scattering cross section as a function of collision energy will indicate the occurrence of a bound state in continuum (BIC). We prove that the minimum will occur at an energy at which the BIC is formed. We discuss how a BIC will be useful for efficient creation of Feshbach molecules and manipulation of cold collisions. Experimental realizations of BIC will pave the way for a new kind of bound-bound spectroscopy in ultracold atoms.

PACS numbers: 03.65.Ge,03.65.Nk,32.80.Qk,34.50.Rk
I. INTRODUCTION

First introduced by von Neuman and Wigner more than eighty years ago [1], a bound state in continuum (BIC) is a counter-intuitive and fundamentally profound concept. The original theoretical approach of Neuman and Wigner has undergone extensions and modifications over the years [2–4]. In recent times, it has attracted renewed research interests [5] with prospective applications in many areas [6–10]. A BIC refers to a discreet eigenstate with energy eigenvalue above the threshold of the continuum of a potential. The amplitude of the wave function of this state falls off in space and so the wave function is square-integrable. Normally, the eigenstates of a one-particle or a multi-particle system above the continuum are infinitely extended and sinusoidal at distances larger than the range of the potential. Below the threshold, there exists negative-energy spectrum of discrete square-integrable bound states. The idea of von Neuman and Wigner was to assume first the existence of a positive-energy square-integrable wave function with its envelop decaying in space, and then to construct an appropriate potential that can support such states. Physically, a BIC occurs due to destructive interference of the outgoing Schrödinger waves scattered by the potential, creating an “unusual” trap [5] for an electron [1]. Hsu et al. [10] have observed trapped light, namely, a BIC of radiation modes by the destructive interference of outgoing radiations amplitudes.

Nearly forty five years after its discovery [1], Stillinger and Herrick [3] extended the idea of BIC to two-body interactions, and discussed its applications in atomic and molecular physics. For two interacting particles, a BIC can be identified with a scattering resonance state with zero width. In general, a resonance at finite energies arises due to the existence of a quasi-bound (almost bound) state at positive energy. In the absence of any other source of dissipation, it is the coupling of the quasi-bound state with the continuum of scattering states that results in finite width of the resonance. This means that zero width of the resonance would imply decoupling of the quasi-bound state from the continuum of scattering states. In other words, the resonance state with zero width becomes a BIC [2, 4].

Here we show that it is possible to create a BIC in cold atom-atom collisions in the presence of two photoassociation (PA) lasers near a magnetic field-induced Feshbach resonance. Our proposed scheme is depicted in Fig.1. The two lasers $L_1$ and $L_2$ are tuned near to the resonance of two excited molecular (bound) states $|b_1\rangle$ and $|b_2\rangle$, respectively. We consider a magnetic Feshbach resonance of two colliding ground-state atoms with two ground-state channels of which
one is closed and the other open. In the absence of coupling with the open-channel, the closed channel is assumed to support a bound state $|b_c⟩$. The two PA lasers couple open-channel continuum of scattering states $|E⟩_{bare}$ with $E$ being collision energy, and $|b_c⟩$ to both the excited bound states. Using projector operator techniques, we analyze the resolvent operator $(z - \hat{H})^{-1}$ of the Hamiltonian operator $\hat{H}$ and thereby arrive at an effective complex Hamiltonian $\hat{H}_{eff}$ of the three interacting bound states. $\hat{H}_{eff}$ is non-hermitian and its eigenvalues are in general complex. However, as we will demonstrate, under appropriate physical conditions, two of the eigenvalues of the effective Hamiltonian can be made real. We establish the mathematical relations involving the parameters of our model that should hold good for the existence of the real eigenvalues. The eigenvectors corresponding to the real eigenvalues are non-decaying states and hence represent bound states in continuum. Similar effective Hamiltonians and their eigenvalue spectrum were studied in the context of two-photon dressed atomic continuum or autoionizing states [11–13] in 1980s. In passing, we would like to mention that non-hermitian Hamiltonians with real eigenvalues also arise in other areas such parity-time (PT) symmetric Hamiltonian systems [14, 15] and Friedrichs-Fano-Anderson model [16–18] where similar spectral singularity appears and can be associated with a non-decaying state in continuum [19, 20].

Here we emphasize that it is possible to detect the two predicted bound states in continuum by two spectroscopic methods, namely photoassociative absorption and photoassociative ionization techniques. Mathematically, a BIC in our model appears as a spectral singularity in the scattering cross section as a function of energy. The expressions of photoassociation probability of either excited bound states as well as the scattering cross section involve the inverse operator $(E - \hat{H}_{eff})^{-1}$. This means that for a real eigenvalue of $\hat{H}_{eff}$ the denominator of the expressions goes to zero. This leads to divergence in scattering cross section implying the occurrence of a resonance with zero width [2, 4], that is, a BIC. However, photoassociative absorption spectrum does not diverge for a real eigenvalue, because the numerator of the expression for the spectrum also goes to zero for the real eigenvalue canceling out the singularity of $(E - \hat{H}_{eff})^{-1}$. Physically, the singularity in scattering cross section implies that BIC is a non-decaying state and hence decoupled from the continuum. However, BIC can make transition to either of the excited bound state via BIC-bound coupling leading to a finite probability for the absorption of a photon. Practically, spectral singularity can not be observed in an experiment. Instead, the signature of BIC will be manifested as an ultra narrow in the coherent photoassociative spectrum or scattering cross section when the collision energy is tuned very close to the energy of the BIC. Usually, photoassociation
is described in terms of atom loss from traps, due to the formation of excited diatomic molecules decaying into two hot atoms or to a diatom that can escape from trap. The occurrence of the bound states in continuum in cold collisions will facilitate to photoassociate two atoms effectively through a bound-bound transition process which can be coherent. We show that a possible signature of a BIC in photoassociative cold collisions appears as a sharp and asymmetric line in photoassociative absorption spectrum as a function of collision energy. Close to the sharp spike-like line, there lies a minimum which resembles to well-known Fano minimum [17] and corresponds to the energy of the BIC.

We further demonstrate that, when the intensities and the detuning parameters of $L_1$ and $L_2$ are adjusted appropriately, one of the bound states in continuum can be reduced to a superposition of $|b_1\rangle$ and $|b_2\rangle$ only while the other BIC results from superposition of all three bound states. We call the first one as A-type BIC and the second one as B-type BIC. The existence of A-type BIC can be probed by a probe laser producing the molecular ion and measuring the ion yield as a function of laser frequency. When the two continuum-bound couplings are much larger than the Feshbach resonance linewidth, the superposition coefficient of $|b_c\rangle$ state in B-type BIC is much larger than those of $|b_1\rangle$ and $|b_2\rangle$. Since the state $|b_c\rangle$ has a magnetic moment, B-type BIC can be probed by bound-free or bound-bound radio-frequency spectroscopy. In case of bound-free spectra, the final state would be two free atoms, and thus B-type BIC can be used for controlling collisional properties of cold atoms. Furthermore, Feshbach molecules can be created by stimulating bound-bound transitions with a radio-frequency pulse at a fixed magnetic field strength. To create Feshbach molecules, the usual method uses a sudden sweep of magnetic field from large negative to large positive scattering length sides of the Feshbach resonance. However, this sudden sweep of magnetic field leads to substantial atom loss due to increase of kinetic energy and thereby limits the atom-molecule conversion efficiency. In contrast, since a BIC is effectively decoupled from the continuum, by creating a B-type BIC, Feshbach molecules can be produced efficiently by inducing stimulated transitions from the BIC to Feshbach molecular states with a radio-frequency pulse.

We also show that, when the coupling of the continuum to one the bound states is turned off, one can still find one BIC which can be identified as the familiar “dark state” made of superposition of the two remaining bound states. Coherent population trapping occurs in this superposition state resulting in the vanishing of the probability of the continuum of scattering states. When laser coupling to either of the excited states is turned off, the model reduces to one [21] that describes
Feshbach resonance-induced Fano effect in photoassociation. The effective Hamiltonian approach
to this model shows that the BIC appears at an energy at which Fano minimum occurs. This can be
identified with the standard result that the population trapping occurs due to the “confluence” of
coherences \( [22] \) at Fano minimum. When the quasibound state in ground-state potential is absent
or the magnetic Feshbach resonance is turned off, the resulting effective Hamiltonian has a real
eigenvalue when the corresponding eigenvector is an excited molecular dark state \( [23] \).

The paper is organized in the following way. In Secs. II and III, we present our model and its
solution, respectively. We analyze in some detail how to realize our model and its application in
cold atoms and molecules in Sec. IV. Finally, we discuss important conclusions of our study in
Sec. V.

II. THE MODEL

The model is schematically depicted in Fig.1. To begin with, we keep our model most general.
Suppose a two-channel model is capable of describing an \( s \)-wave Feshbach resonance in ground-
state atom-atom cold collision. One of these two channels is open and the other is closed. The
closed channel is assumed to support a bound state \( | b_c \rangle \). The thresholds of these two ground-state
channels and the binding energy of \( | b_c \rangle \) are tunable with an external magnetic field. Both the bare
continuum of scattering states \( | E \rangle_{\text{bare}} \) in the open channel with \( E \) being the collision energy, and
\( | b_c \rangle \) are coupled to two bound states \( | b_1 \rangle \) and \( | b_2 \rangle \) in an excited molecular potential by two lasers
\( L_1 \) and \( L_2 \), respectively. Suppose, the states \( | b_1 \rangle \) and \( | b_2 \rangle \) have same rotational quantum numbers
\( J_1 = J_2 = 1 \), but they have different vibrational quantum numbers if both of them are supported
by the same adiabatic molecular potential. In case they belong to different molecular potentials,
their vibrational quantum numbers may be same or different. The energy spacing between \( | b_1 \rangle \)
and \( | b_2 \rangle \) is assumed to be large enough compared to the line widths of the two lasers. Furthermore,
\( | b_1 \rangle \) and \( | b_2 \rangle \) are assumed to be far below the dissociation threshold of excited potential(s) so that
the transition probability at the single-atom level be negligible.

In the rotating wave approximation, the Hamiltonian of our mode can be expressed as \( \hat{H} = \hat{H}_0 + \hat{V} \) where

\[
\hat{H}_0 = \sum_n \left( E_n - \hbar \omega_{L_n} \right) | b_n \rangle \langle b_n | + E_0 | b_c \rangle \langle b_c | + \int E'dE' | E' \rangle_{\text{bare}} \langle E' | \tag{1}
\]
FIG. 1: A schematic diagram for creating BIC in ultracold atoms. Two lasers $L_1$ and $L_2$ are used to excite PA transitions from the magnetic Feshbach-resonant collisional state of two ultracold ground-state ($S + S$) atoms to the two bound states $b_1$ and $b_2$, respectively, in the same electronically excited molecular potential. The magnetic Feshbach resonance is considered as a two-channel model in the electronic ground-state potentials with the lower channel being open and the upper one being closed. In the large separation limit the ground-state channel potential corresponds to two separated $S + S$ atoms while the excited-state potential connects to two separated $S + P$ atoms.

\[
\hat{V} = \sum_n \int dE' \Lambda_n(E') \langle b_n \rangle_{\text{bare}} E' \langle b_c \rangle_{\text{bare}} E' + \int dE' V_{E'} \langle b_c \rangle_{\text{bare}} E' + \sum_n \hbar \Omega_n \langle b_n \rangle \langle b_c \rangle + \text{C.c.}
\]

$E_n$ is the binding energy of $n$-th excited molecular state $\langle b_n \rangle$, $\omega_{L_n}$ denotes the frequency of the $L_n$ laser, $E_c$ being the energy of the closed channel bound state $\langle b_c \rangle$ and $| E' \rangle_{\text{bare}}$ the bare continuum of scattering state with energy $E'$. Note that all the energies are measured from the open channel threshold unless stated otherwise. Here $\Lambda_n(E)$ is the dipole matrix element of transition $| E \rangle_{\text{bare}} \rightarrow | b_n \rangle$, $V_E$ is the coupling between the closed channel bound state $| b_c \rangle$ and the open channel scattering state $| E \rangle_{\text{bare}}$, and $\Omega_n$ is the Rabi frequency between $| b_n \rangle$ and $| b_c \rangle$. The magnetic Feshbach resonance linewidth is $\Gamma_f = 2\pi |V_E|^2$. 

\[
\hat{V} = \sum_n \int dE' \Lambda_n(E') \langle b_n \rangle_{\text{bare}} E' \langle b_c \rangle_{\text{bare}} E' + \int dE' V_{E'} \langle b_c \rangle_{\text{bare}} E' + \sum_n \hbar \Omega_n \langle b_n \rangle \langle b_c \rangle + \text{C.c.}
\]
To study BIC, we analyze the resolvent operator \( G(z) = (z - \hat{H})^{-1} \) and introduce the projection operators

\[
P = |b_c\rangle\langle b_c| + \sum_{n=1,2} |b_n\rangle\langle b_n|
\]

\[
Q = 1 - P = \int dE |E\rangle_{\text{bare}}\langle E|
\]

which satisfy the properties

\[
PP = P, \quad QQ = Q, \quad PQ = QP = 0, \quad P + Q = 1
\]

Thus we have

\[
G = G_0 + G_0\hat{V}G = \frac{1}{E - \hat{H}_0 + i\epsilon} + \frac{1}{E - \hat{H}_0 + i\epsilon}\hat{V}G
\]

Projecting out the bare continuum states, after some algebra as given in appendix-A, we obtain an effective Hamiltonian of interacting three bound states. Explicitly, this Hamiltonian is given by

\[
H_{\text{eff}} = H_0 + \sum_{n,n'=1,2} \left[ \left( \hbar\delta_{nn'} - \frac{i\hbar\Gamma_{nn'}(E)}{2} \right) |b_n\rangle\langle b_{n'}| + \left( \delta_{c} - \frac{i\hbar\Gamma_{f}(E)}{2} \right) |b_{c}\rangle\langle b_{c}| + \right.
\]

\[
+ \sum_n \frac{\hbar\Gamma_{nf}(E)}{2} \{q_{nf} - i\} |n\rangle\langle b_{c}| \left. + \text{C.c.} \right]
\]

where \( \delta_{nn} = (E_n + \Delta_{nn}^{\text{shift}})/\hbar - \omega_{L_n} \) is the detuning of the light-shifted \( n \)th excited level from the \( L_n \) laser frequency \( \omega_{L_n} \), \( \delta_{nn'} = \hbar^{-1}\Delta_{nn'}^{\text{shift}} \) \( (n \neq n') \), where \( \Delta_{nn'}^{\text{shift}} \) is the real part of the quantity \( \int dE' \Lambda_n^*(E') \Lambda_{n'}(E')/(E - E') \) between, \( \Gamma_{nn'}(E) = 2\pi\Lambda_n^*(E)\Lambda_{n'}(E) \). Here \( \delta_{c} = \hbar^{-1} [E_c(B) + \Delta_f^{\text{shift}} - E_{\text{th}}(B)] \) is the detuning of the shifted closed channel bound state level from the the threshold \( E_{\text{th}} \) of the open channel. Note that \( \delta_{c} \) is a function of the applied magnetic field \( B \) due to the dependence of \( E_c \) and \( E_{\text{th}} \) on \( B \). \( \Delta_f^{\text{shift}} = \mathcal{P} \int dE'|V_{E'}|^2/(E - E') \), where \( \mathcal{P} \) stands for Cauchy’s principal value, is the shift due to magnetic coupling \( V_{E'} \) between \( |b_{c}\rangle \) and \( |E'\rangle_{\text{bare}} \). \( q_{nf} \) is the well-known Fano-Feshbach asymmetry parameter defined by

\[
q_{nf} = \frac{\delta_{nf}^{\text{shift}} + \Omega_n}{\Gamma_{nf}/2}.
\]
where $\Omega_n$ is the Rabi frequency for transition $|b_c\rangle \leftrightarrow |b_n\rangle$ and

$$\delta_{nf}^\text{shift} = \hbar^{-1} \mathcal{P} \int dE' \Lambda_n^*(E') V_{E'}/(E - E')$$

(9)

is a frequency-shift of $|b_c\rangle \leftrightarrow |b_n\rangle$ transition frequency due to the indirect coupling of the two bound states via the continuum. Here $\Gamma_{nf} = 2\pi \hbar^{-1} \Lambda_n^*(E)V_{E'}$. For energy $E$ near the threshold of the continuum, the region $E' > E$ of the above integrand contributes more strongly [24]. As a result, $\delta_{nf}^\text{shift}$ will be negative at low energy. Since $\Omega_n$ is positive, the sign of $q_{nf}$ depends on the relative strength between $|\delta_{nf}^\text{shift}|$ and $\Omega_n$. Since the magnetic coupling $V_{E'}$ is determined by the hyperfine spin coupling between the closed and the open channel, its value depends on the specific atomic system chosen. In contrast, the laser couplings $\Omega_n$ and $\delta_{nf}^\text{shift}$ depend on which bound state $|b_n\rangle$ is chosen for the laser to be tuned to, in accordance with Franck-Condon principle of molecular spectroscopy. Thus, it is possible to alter the sign and magnitude of Fano-Feshbach asymmetry parameter in our model through the selectivity of the excited molecular bound states. Since in molecular excited states, there is a host of vibrational levels in different molecular symmetries that can be accessed by PA, there is a lot of flexibility in choosing the excited bound states in our model. We will further discuss this point in Sec.IV.

In the absence of the lasers fields, the magnetic field-dependent resonant scattering phase shift $\eta_r$ and the s-wave scattering length $a_s$ are given by

$$-\cot \eta_r = \frac{E - \tilde{E}_c}{\hbar \Gamma_f/2} \simeq \frac{1}{ka_s} + \frac{1}{2} r_0 k$$

(10)

$\tilde{E} = E_c + \Delta_f^\text{shift}$ is the shifted energy of $|b_c\rangle$, $k$ is the wave number related to the collision energy $E = \hbar^2 k^2 / 2\mu$ with $\mu$ being the reduced mass of the two colliding atoms. Here $r_0$ is the effective range of the open-channel ground-state potential. In the limit $k \to 0$, $\Gamma_f/2 \simeq kG_f$ where $G_f$ is a constant having the dimension L s$^{-1}$. The scattering length $a_s$ and the effective range $r_0$ are related to $\tilde{E}_c$ and $G_f$ by $a_s = \frac{\tilde{E}_c}{\hbar G_f}$ and $r_0 = \frac{\hbar}{\mu G_f}$, respectively. This means the magnetic field dependent detuning $\delta_c(B) = -G_f/a_s$. When $\tilde{E}_c > 0$, $a_s$ is negative and the $|b_c\rangle$ lies above the threshold of the open channel and hence $|b_c\rangle$ is a quasi-bound state. In contrast, when $\tilde{E}_c < 0$, $|b_c\rangle$ is a true bound state (Feshbach molecular state) and scattering length is positive. Later, we will show that by forming a BIC with large scattering length, the BIC can be converted into a Feshbach molecule by stimulated radio-frequency spectroscopy.
III. THE SOLUTION

For simplicity, let us introduce the dimensionless parameters
\[ \tilde{\delta}_n = \frac{\delta_{nn}}{\Gamma_f/2} \]
\[ g_{nn'} = \frac{\Gamma_{nn'}}{(\Gamma_f/2)} (n \neq n') \]. We assume that \( \delta_{12}^{\text{shift}} = \delta_{21}^{\text{shift}} \simeq 0 \), that is, the real parts of laser-induced couplings between \( |b_1\rangle \) and \( |b_2\rangle \) are negligible. Assuming the two free-bound photoassociative couplings \( \Lambda_{nE} \) to be real quantities, we have \( \Lambda_{nE}V_E/|V_E|^2 = \Lambda_{nE}/V_E = \sqrt{g_n} \)

Under these conditions, the effective Hamiltonian of Eq.(7) can be written in matrix form
\[ H_{\text{eff}} = \frac{\hbar \Gamma_f}{2} [A + iB] \] (11)
where
\[ A = \begin{pmatrix} \tilde{\delta}_1 & 0 & q_{1f}\sqrt{g_1} \\ 0 & \tilde{\delta}_2 & q_{2f}\sqrt{g_2} \\ q_{1f}\sqrt{g_1} & q_{2f}\sqrt{g_2} & - (ka_s)^{-1} \end{pmatrix} \] (12)
and
\[ B = \begin{pmatrix} -g_1 & -g_{12} & -\sqrt{g_1} \\ -g_{21} & -g_2 & -\sqrt{g_2} \\ -\sqrt{g_1} & -\sqrt{g_2} & -1 \end{pmatrix} \] (13)

For \( (ka_s)^{-1} = 0 \), these matrices have the same form as the Eq. (2.18) of Ref.[13]. The secular equation for B matrix is \( x^3 + (g_1 + g_2 + 1)x^2 = 0 \) and it has two roots equal to zero and the third one equal to \(- (g_1 + g_2 + 1)\). When the two eigenvectors of B with zero eigenvalues become simultaneous eigenvectors of A with real eigenvalues, we have two real roots of the effective Hamiltonian. In addition, when A and B commute, both these matrices are diagonalizable within simultaneous eigenspace, with \( H_{\text{eff}} \) having two real eigenvalues. The commutative condition can be easily found to be
\[ q_{1f} + \tilde{\delta}_1 = q_{2f} + \tilde{\delta}_2 = q_{1f}g_1 + q_{2f}g_2 - (ka_s)^{-1} \] (14)

To evaluate the two real eigenvalues of the complex Hamiltonian \( H_{\text{eff}} \), we proceed in the following way. We first get an eigenvector of the matrix A with an unknown eigenvalue \( \lambda \) in the form
\[ X = C \begin{pmatrix} 1 \\ x_2 \\ x_3 \end{pmatrix} \] (15)
where $C$ is normalization constant and $x_2$ and $x_3$ are the two elements of the vector. All these three quantities $C$, $x_2$ and $x_3$ are the functions of $\lambda$. Assuming that $X$ is also an eigenvector of $B$ with zero eigenvalue, the eigenvalue equation $BX = 0$ leads to a quadratic equation for $\lambda$, the solutions of which are the desired eigenvalues. For zero eigenvalue, the eigenvalue equation quantities 

By expressing $\delta_2$ and $g_1$ cannot be arbitrary when $H_{eff}$ has the real eigenvalues. By expressing $x_2$, $x_3$ and $C$ in terms of the set of the parameters $g_2$, $\tilde{\delta}_2$, $q_{1f}$ and $q_{2f}$, from the eigenvalue equation $AX = \lambda X$ one obtains 

with $\lambda \neq \tilde{\delta}_2$. Now, replacing $\lambda$ by a real eigenvalue of Eq. (16), one can use the above equation to set the appropriate parameter space of $g_1$ and $\tilde{\delta}_1$ for which $\lambda$ remains real and fixed for a fixed set of other parameters.

Let us now consider the special case of both excited bound states belonging to the same excited molecular potential with closely lying vibrational quantum numbers $1 \leq |v_1 - v_2| \leq 2$. Hence, the bound-bound Franck-Condon (FC) factors for transitions $| b_c \rangle \leftrightarrow | b_1 \rangle$ and $| b_c \rangle \leftrightarrow | b_2 \rangle$ will be nearly equal. Similarly, the free-bound FC factors for transitions $| E \rangle_{bare} \leftrightarrow | b_1 \rangle$ and $| E \rangle_{bare} \leftrightarrow | b_2 \rangle$ will also be almost equal. Since Fano asymmetry parameters $q_{1f}$ and $q_{2f}$ are independent of laser intensities, but are dependent of these FC factors, we expect $q_{1f} \approx q_{2f}$. The BIC condition of Eq. (14) then implies $\tilde{\delta}_1 = \tilde{\delta}_2$. Now, putting $q_{1f} = q_{2f} = q_f$, the commutativity condition implies $\tilde{\delta}_1 = \tilde{\delta}_2 = q_f(g_1 + g_2 - 1)$. Under these conditions, two real roots of the effective Hamiltonian are 

$$E_A = \frac{\hbar \Gamma_f}{2} \lambda_+ = \frac{\hbar \Gamma_f}{2} q_f(g_1 + g_2 - 1)$$

$$E_B = \frac{\hbar \Gamma_f}{2} \lambda_- = -\frac{\hbar \Gamma_f}{2} q_f$$

(18)
The BIC state corresponding to \( E_A \) is

\[
| A \rangle_{\text{BIC}} = \frac{1}{\sqrt{g_1 + g_2}} \left[ \sqrt{g_2} | b_1 \rangle - \sqrt{g_1} | b_2 \rangle \right] \tag{20}
\]

Note that this state does not mix with the closed channel bound state \( | b_c \rangle \), and so this eigenvector is immune to magnetic field tuning of the Feshbach resonance. Nevertheless, \( | b_1 \rangle \) and \( | b_2 \rangle \) remain coupled with \( | b_c \rangle \) and \( | E \rangle_{\text{bare}} \) due to the lasers. It is easy to see that the photoassociative transition matrix element for the interaction Hamiltonian

\[
\hat{V}_{PA} = \sqrt{g_1} | b_1 \rangle_{\text{bare}} \langle E | + \sqrt{g_2} | b_2 \rangle_{\text{bare}} \langle E | + \text{C.c. between} | E \rangle_{\text{bare}} \text{ and } | A \rangle_{\text{BIC}} \text{ is zero. This means that this is an excited molecular dark state that is predicted to play an important role in suppression of photoassociative atom loss} \[23]. \]

We call this dark state as A-type BIC. The eigenstate corresponding to the eigenvalue \( E_B \) is given by

\[
| B \rangle_{\text{BIC}} = \left[ \frac{1}{(g_1 + g_2)(g_1 + g_2 + 1)} \right]^{\frac{1}{2}} \left[ \sqrt{g_1} | b_1 \rangle + \sqrt{g_2} | b_2 \rangle + (g_1 + g_2) | b_c \rangle \right] \tag{21}
\]

This is a superposition of all three bound states. The involvement of \( | b_c \rangle \) makes this BIC dependent on the magnetic field \( B \). We call this state as B-type BIC. Near unitarity regime, \( |ka_s| \) is large and consequently \( |(ka_s)^{-1}| \ll 1 \), and hence the effect of finite \( (ka_s)^{-1} \) can be taken into account perturbatively. The perturbation part of the Hamiltonian is then \( V = -\frac{\hbar \Gamma_f}{2} (ka_s)^{-1} | b_c \rangle \langle b_c | \), and the first order correction to the energy \( E_B \) is given by

\[
\Delta E_B = _{\text{BIC}}\langle B | V | B \rangle_{\text{BIC}} = -\frac{\hbar \Gamma_f}{2} (ka_s)^{-1} \frac{g_1 + g_2}{g_1 + g_2 + 1} \tag{22}
\]

The signature of this BIC can be detected in a number of coherent spectroscopic methods as will be discussed in the next section. For example, a BIC may be manifested as a strong and narrow photoassociative absorption line.

IV. APPLICATIONS: RESULTS AND DISCUSSIONS

Before we discuss some specific applications, it is worthwhile to make some general observations on the dependence of the two real eigenvalues \( E_A \) and \( E_B \) on the magnetic field tuning of Feshbach resonance. In the zero energy limit \( (E \to 0) \) and near the vicinity of Feshbach resonance, the applied magnetic field \( B \) and the scattering length \( a_s \) are related by

\[
a_s^{-1} = -a_{bg}^{-1} \left( \frac{B - B_0}{\Delta} \right) \tag{23}
\]

where \( B_0 \) is the resonance magnetic field at which \( a_s \to \infty \) and \( a_{bg} \) is the background scattering length. Since \( a_{bg} \Delta > 0 \), \( a_s < 0 \) for \( B > B_0 \) and \( a_s > 0 \) for \( B < B_0 \). In case of Fermionic
atoms, $B > B_0 \ (B < B_0)$ region is commonly known as BCS (BEC) side of the resonance. The parameter range $-1.0 \leq (ka_s)^{-1} \leq 1.0$ is usually referred to as ‘unitarity’ regime.

Though $E_A$ changes with the change of $(ka_s)^{-1}$, the corresponding eigenstate of Eq. (20) remains intact and so coherent population trapping occurs (CPT) in A-type BIC that remains protected against the tuning of magnetic field or the scattering length. In contrast, both eigenvalue and eigenstate of B-type BIC depends on $B$ or $a_s$. For $a_s \to \infty$ and $g_1 + g_2 > 1$, as $q_f \to \pm 0$, $E_A \to \pm 0$ and $E_B \to \mp 0$ as can be inferred from the expressions (18) and (19). Note that the eigenvalues of both A- and B-type BIC depend inversely on $ka_s$.

A. Detection of BIC via photoassociation

Modifications of photoassociation probability as a result of the formation of BIC can be ascertained by making use of isometric and invertible Møller operators $\Omega_{\pm}$ of scattering theory. Since before turning on the lasers and the magnetic field, the atoms are in a resonant collisional state, incoming state of the problem can be taken to be the bare continuum $|E\rangle_{\text{bare}}$. The dressed continuum state $|E+\rangle$ is given by

$$|E+\rangle = \Omega_+ |E\rangle_{\text{bare}}$$  \hspace{1cm} (24)

where

$$\Omega_+ = 1 + G(z + i\epsilon)V$$  \hspace{1cm} (25)

The probability of photoassociative transition $|E\rangle \to |b_n\rangle$ is given by

$$P_n = \int dE |\langle b_n | E+\rangle|^2$$  \hspace{1cm} (26)

The quantity

$$S_n(E) = |\langle b_n | E+\rangle|^2$$  \hspace{1cm} (27)

is the photoassociation probability per unit collision energy. Now, we have

$$\langle b_n | E+ \rangle = \langle b_n | (P + Q)G(z + i\epsilon)(P + Q)V | E\rangle$$

$$= \langle b_n | PG(z + i\epsilon)(P + Q)V | E\rangle_{\text{bare}}$$  \hspace{1cm} (28)
Using Eq. (A.3) we have

\[ \begin{align*}
PGQ &= P(Q + GPVQ) \frac{1}{E - H_0 - VQ + i\epsilon} \\
&= PGPVQ \frac{1}{E - H_0 - VQ + i\epsilon} 
\end{align*} \]

(29)

\[ \langle b_n \mid \Omega_+ \mid E \rangle_{\text{bare}} = \langle b_n \mid PG(E + i\epsilon)PR(E + i\epsilon) \mid E \rangle_{\text{bare}} \]

(30)

where \( R(E + i\epsilon) \) is given in Eq. (A5). Now,

\[ PG(E + i\epsilon)P = (E - H_{\text{eff}} + i\epsilon)^{-1} = \frac{2}{\hbar \Gamma_f \text{Det}[(\tilde{E} - \tilde{H}_{\text{eff}})]} \text{\mathcal{A}} \]

(31)

where \( \tilde{E} = 2E/\hbar \Gamma_f, \tilde{H}_{\text{eff}} = A + iB \) and \( \mathcal{A} \) is the transpose of the co-factor matrix of \( (\tilde{E} - \tilde{H}_{\text{eff}}) \).

Thus we have

\[ \langle b_n \mid \Omega_+ \mid E \rangle = \sqrt{\frac{2}{\pi \hbar \Gamma_f \text{Det}[(\tilde{E} - \tilde{H}_{\text{eff}})]}} \sum_{m=1,2} \mathcal{A}_{mn} \sqrt{g_m + \mathcal{A}_{n3}} \]

(32)

The quantity within the third bracket in the numerator of the above equation, for \( n = 1 \) and \( (k\alpha_s)^{-1} = 0 \), can be expressed as

\[
\begin{align*}
- \sqrt{g_1} &\left[ -\tilde{E}(\tilde{\delta}_2 - \tilde{E}) - g_2q_{2f}^2 - i(\tilde{\delta}_2 - \tilde{E}) + ig_2q_{2f} + ig_2q_{2f} \right] \\
+ \sqrt{g_2} &\left[ -q_{1f}q_{2f}\sqrt{g_1g_2} + i\sqrt{g_1g_2}(q_{1f} + q_{2f}) + i\sqrt{g_1g_2}\tilde{E} \right] \\
- \left[ -q_{1f}\sqrt{g_1}(\tilde{\delta}_2 - \tilde{E}) - ig_2\sqrt{g_1}q_{2f} + ig_2\sqrt{g_1}q_{1f} + i\sqrt{g_1}(\tilde{\delta}_2 - \tilde{E}) \right]
\end{align*}
\]

(33)

the zeros of which are the roots of the quadratic equation

\[ \tilde{E}(\tilde{\delta}_2 - \tilde{E}) + g_2q_{2f}^2 - q_{1f}q_{2f}g_2 + q_{1f}(\tilde{\delta}_2 - \tilde{E}) = 0 \]

(34)

Thus, the numerator has two zeros at

\[ \tilde{E}_\pm = \tilde{\delta}_2 + \frac{1}{2} \left[ -(\tilde{\delta}_2 + q_{1f}) \pm \sqrt{(\tilde{\delta}_2 + q_{1f})^2 + 4q_{2f}g_2(q_{2f} - q_{1f})} \right] \]

(35)

It is important to note that the two zeros of the numerator are the same as the two real eigenvalues of \( H_{\text{eff}} \) as given in Eq. (16). This means that, although the denominator

\[ \text{Det} \left[ \tilde{E} - \tilde{H}_{\text{eff}} \right] = \sum_{i=1}^{3} (\tilde{E} - \tilde{E}_i) \]

(36)
FIG. 2: Dimensionless spectrum $S_1(E)/E_f$ as a function of dimensionless energy $E/E_f$ (where $E_f = \hbar \Gamma_f/2$) for $g_1 = 0.25$ (solid), $g_1 = 0.5$ (dashed) and $g_1 = 0.75$ (dashed-dotted) with $q_{1f} = -0.5$, $q_{2f} = -1.0$, $g_2 = 2.0$, $\tilde{\delta}_2 = -0.5$ and $\tilde{\delta}_1 = 1.5$. For the solid curve the three complex eigenvalues of $\tilde{H}_{\text{eff}}$ are $\tilde{E}_1 = 1.0964 - 0.0010i$, $\tilde{E}_2 = 1.4989 - 0.0992i$, and $\tilde{E}_3 = -1.5953 - 3.1498i$; for dashed curve $\tilde{E}_1 = 1.0242 - 0.0164i$, $\tilde{E}_2 = 1.4862 - 0.1653i$, and $\tilde{E}_3 = -1.5104 - 3.3184i$; for dashed-dotted curve $\tilde{E}_1 = 0.9581 - 0.0421i$, $\tilde{E}_2 = 1.4645 - 0.2111i$, and $\tilde{E}_3 = -1.4226 - 3.4968i$. When $g_1 = 0.1803$, $\tilde{E}_1$ becomes real and is equal to 1.1180 which correspond to the minimum of the spectral lines. The spike height of the solid curve is $2.2 \times 10^4$.

where $\tilde{E}_i$ represents an eigenvalue of $\tilde{H}_{\text{eff}}$, may become zero for a real eigenvalue of $\tilde{H}_{\text{eff}}$, the spectrum remains finite in the limit $\tilde{E} \to \tilde{E}_i$ for a real eigenvalue $\tilde{E}_i \equiv \lambda_{\pm}$. When the real part of a complex eigenvalue is nearly equal to a real eigenvalue, and the imaginary part is extremely small ($\ll \hbar \Gamma_f$), the spectrum $S(E)$ as a function of collision energy $E$ will exhibit Fano-like minimum and a highly prominent maximum lying close to the minimum. Experimentally, searching for such a spectral structure is possible by choosing the parameters $\tilde{\delta}_2$, $g_2$, $q_{1f}$ and $q_{2f}$ for a zero of the numerator, but $g_1$ and $\tilde{\delta}_1$ are chosen such that the real part of one of the eigenvalues of $H_{\text{eff}}$ is nearly equal to a zero of the numerator with the imaginary part being small. A Fano-like spectral structure with a nearby narrow spectral spike will indicate the existence of BIC [13].

Figures 2 and 3 display photoassociative absorption spectra $S_1(E)$ (which is a measure of probability of transition to $| b_1 \rangle$) as a function function of $E$ for different values of $g_1$ keeping all other parameters fixed. We scale all energy quantities by $E_f = \hbar \Gamma_f/2$. The fixed parameters are chosen such that they fulfill the Eq. (35). The different values of $g_1$ are chosen close to a value
FIG. 3: Same as in Fig. 2 but for $g_1 = 5.5$ (solid), $g_1 = 5.0$ (dashed) and $g_1 = 4.5$ (dashed-dotted) with fixed parameters $q_{1f} = 0.5, q_{2f} = 1.0, g_2 = 5.0, \delta_1 = 1.45$ and $\delta_2 = -1.5$. For solid curve the eigenvalues are $\tilde{E}_1 = 0.6645 - 4.5 \times 10^{-6}i$, $\tilde{E}_2 = -2.2178 - 0.4279i$, and $\tilde{E}_3 = 1.55338 - 11.0720i$; for dashed curve $\tilde{E}_1 = 0.7036 - 0.0002i$, $\tilde{E}_2 = -2.2165 - 0.44027i$, and $\tilde{E}_3 = 1.51292 - 10.5595i$; for dashed-dotted curve $\tilde{E}_1 = 0.7466 - 0.0008i$, $\tilde{E}_2 = -2.2153 - 0.4534i$, and $\tilde{E}_3 = 1.4687 - 10.0457i$. For $g_1 = 5.2516$, $\tilde{E}_1$ is real and equal to 0.6583. The spike height of the solid curve is $1.0 \times 10^6$.

...that is given by the condition (17) for the occurrence of a real eigenvalue $\lambda = \tilde{E}_x$ for the given $\delta_1$. The results displayed in Figs. 2 and 3 and the data mentioned in the figure captions clearly support our analytical results described above. The spikes in solid curves occur due to the BIC with real eigenvalue close to the real part of $\tilde{E}_1$. In Fig. 2, the bumps near $E = 1.5E_f$ occurs due to the complex eigenvalue $\tilde{E}_2$. Note that, as can be seen from the Eq.(8), the Fano-Feshbach asymmetry parameter will be positive (negative) when the Rabi frequency $\Omega$ is greater (smaller) than the magnitude $\delta_{nf}^{\text{shift}}$ which is negative.

B. Possible realizations of the model

We next discuss the possibility of experimental realization of our model in ultracold atomic gases that are of current experimental interests. The discussed BIC can be realized in ultracold atoms with currently available experimental techniques of magnetic Feshabch resonances [25] and photoassociation [26, 27]. In particular, our theoretical proposal can be implemented in case of experimentally observed narrow Feshbach resonances in cold alkali atoms like $^{23}\text{Na}$ [28–33].
are preferable since the life-time of the quasi-bound state in such resonances will be appreciable for the lasers to excite bound-bound transitions. For $|\chi\rangle \leftrightarrow |b_n\rangle$ bound-bound laser coupling $\Omega_n$ to be significant, one needs to choose the excited bound state $|b_n\rangle$ such that its outer turning point lies within an intermediate separation $r (20 \leq r \leq 30)$, since the wavefunction of $|\chi\rangle$ is usually peaked in this range. It is possible to find such excited bound states of alkali dimers having outer turning points at such intermediate separations, and such bound state are accessible by PA transitions as demonstrated in a number of experiments.

As an example, let us consider narrow Feshbach resonance in ultracold $^{87}$Rb atomic gas near magnetic field strength 1007.4 G [35, 36] in order to realize BIC in cold collisions. This resonance is characterized by the parameters: zero crossing width $\Delta = 0.21$ G, background scattering length $a_{bg} = 100.5a_0$, the difference between magnetic moments of the closed-channel bound state $|b_c\rangle$ and the two free atoms is $\delta\mu = 2.79\mu_B$, where $\mu_B$ is Bohr magnetron. This means the Feshbach resonance linewidth $\Gamma_f = k a_{bg} \Delta \delta\mu$ where $k$ is the collision wave number related to the collision energy $E = \hbar^2 k^2/(2\mu)$ with $\mu$ being the reduced mass of the two atoms. For $E = 50$ nK, $\Gamma_f \sim 10$ kHz. The values of parameters $g_1$ and $g_2$ used in Figs. 2 and 3 would correspond to stimulated line widths of the order of 10 or 100 kHz. From the positions of the minimum in Figs. 2 and 3, it may be noted that BIC will occur at sub-$\mu$K energy, requiring Bose-Einstein condensate of $^{87}$Rb atoms in order to realize a BIC near this particular Feshbach resonance. However, the theoretical results depicted in Figs. 2 and 3 can fit into several other alkali atoms for which a condensate is not essential. Moreover, different parameter regimes can be used for different alkali systems. In short, our model provides a vast range of parameter space with well defined relationship among the various parameters for searching for BIC in cold collisions.

C. Detection of BIC via photoassociative ionization spectroscopy

BIC can also be detected by photoassociative ionization spectroscopy. In BIC scheme of Fig.1, a third laser $L_3$ can be applied to excite molecular auto-ionization transitions $|A\rangle_{BIC} \rightarrow |b_3\rangle$, where $|b_3\rangle$ represents a bound state in an excited potential that asymptotically corresponds to two atoms in $P + P$ electronic states. Since molecular state $|b_3\rangle$ is made of two doubly excited atoms, it can autoionize to produce molecular ion. Since $|b_1\rangle$ and $|b_2\rangle$ can be chosen to be energetically close, $L_3$ can couple both of them to $|b_3\rangle$. Therefore, we can construct a photoassociative...
ionization (PAI) interaction operator

\[ \hat{V}_{PAI}(t) = \Omega_{31} e^{-i(\omega_{L3} - \omega_{31})t} \langle b_3 | + \Omega_{32} e^{-i(\omega_{L3} - \omega_{32})t} \langle b_3 | b_2 | + C.c \] (37)

where \( \Omega_{31} \) and \( \Omega_{32} \) are the Rabi frequencies for the transitions \( | b_1 \rangle \rightarrow | b_3 \rangle \) and \( | b_2 \rangle \rightarrow | b_3 \rangle \), respectively; \( \omega_{L3} \) is the frequency of \( L_3 \) laser, and \( \omega_{3n} \) is the transition frequency for the transition \( | b_1 \rangle \leftrightarrow | b_3 \rangle \). The PAI spectrum is given by

\[ S_{PAI}(\omega_{L3}) = \left| \int_0^\infty d\tau \int dE e^{-iE\tau/\hbar - \gamma\tau/2} \langle b_3 | \hat{V}_{PAI}(\tau) | E+ \rangle \right|^2 \] (38)

where \( \gamma \) is the non-radiative autoionizing line width of \( | b_3 \rangle \). Using the eigenstates \( | \lambda_i \rangle \) \( (i = 1, 2, 3) \) of \( H_{eff} \), one can employ the identity operator \( \sum_i | \lambda_i \rangle \langle \lambda_i | \) to express \( \langle b_n | E+ \rangle \) in terms of \( | \lambda_i \rangle \) basis

\[ \langle b_n | E+ \rangle = \sum_{i=1}^{3} \frac{\langle b_n | \lambda_i \rangle \langle \lambda_i | V | E \rangle_{\text{bare}}}{E - \lambda_i \hbar \gamma_f/2 + i\epsilon} \] (39)

When BIC conditions for \( g_1f = g_2f = g_f \) are fulfilled, two of the \( \langle \lambda_i \rangle \) are bound states in continuum, of which one is A-type and the other is B-type. For \( g_1 >> 1 \) and \( g_2 >> 1 \), the probability amplitudes of \( | b_1 \rangle \) and \( | b_2 \rangle \) in B-type BIC will be very small. Now, since the operator \( \hat{V}_{PAI} \) couples \( | b_1 \rangle \) and \( | b_2 \rangle \) only to \( | b_3 \rangle \), it is expected that, under the conditions \( g_1 >> 1 \) and \( g_2 >> 1 \), the laser \( L_3 \) will predominantly couple A-type BIC to \( | b_3 \rangle \). Thus PAI spectrum can be approximated as

\[ S_{PAI} \simeq | \langle \text{BIC} | A | V | E \rangle_{\text{bare}} |^2 \times \left| \frac{\Omega_{31} \sqrt{g_2}}{(\omega_{31} - \omega_{\text{BIC}}^A - \omega_{L3}) + i\gamma/2} - \frac{\Omega_{32} \sqrt{g_1}}{(\omega_{32} - \omega_{\text{BIC}}^A - \omega_{L3}) + i\gamma/2} \right|^2 \] (40)

where \( \omega_{\text{BIC}}^A = E_A/\hbar \) is the eigenfrequency of A-type BIC. Clearly, the spectrum will show a shift equal to \( \omega_{\text{BIC}}^A \). The spectral intensity will be suppressed (enhanced) depending on whether the quantity

\[ \text{Re} \left[ \frac{\Omega_{31} \Omega_{32} \sqrt{g_1 g_2}}{(\omega_{31} - \omega_{\text{BIC}}^A - \omega_{L3} + i\gamma/2)(\omega_{32} - \omega_{\text{BIC}}^A - \omega_{L3}) - i\gamma/2} \right] \] (41)

is positive (negative). Thus one can detect A-type BIC by PAI with a probe laser \( (L_3) \) in the presence of two PA lasers and a magnetic field under BIC conditions.
When BIC conditions as discussed in the model and solution sections are fulfilled, the eigenstate with real eigenvalue (i.e., BIC) effectively becomes decoupled from the bare continuum while the optical and the magnetic transitions between the continuum and the bound states remain active. As the system parameters are being tuned very close to the BIC conditions, the complex eigenvalue will tend to become real. The complex eigenvalue with small imaginary part implies the leakage of the probability amplitude of the BIC into the continuum. This will give rise to a resonant structure with extremely narrow width in the variation of the scattering cross section as a function of energy. To calculate the scattering $T$-matrix, we follow the standard method of scattering theory based on Møller operators $\Omega_{\pm}$. The dressed continuum $|E+\rangle$ describes outgoing scattering waves that are influenced by laser light and the magnetic field. The part of the scattering $T$-matrix element that is modified by the two laser fields and the magnetic field is

$$T_{\text{field}}(E) = \text{bare} \langle E | \hat{V} | E+ \rangle = \text{bare} \langle E | \hat{V} \Omega_+ | E \rangle_{\text{bare}}$$

can be written as

$$T_{\text{field}}(E) = \text{bare} \langle E | V(P + Q)G(z + i\epsilon)(P + Q)V | E \rangle_{\text{bare}}$$

(42)

Since $\text{bare} \langle E | VQ = 0$ and $QV \langle E \rangle_{\text{bare}} = 0$, we have $T_{\text{field}}(E) = \text{bare} \langle E | VPGPV | E \rangle_{\text{bare}}$. Now, using the relation $PG(E + i\epsilon)P = (E - H_{\text{eff}} + i\epsilon)^{-1}$ we can express

$$T_{\text{field}}(E) = \frac{1}{\text{Det}[\langle \tilde{E} - \tilde{H}_{\text{eff}} \rangle]} \sum_{n=1}^{3} V_n^*(E) \sum_{m=1}^{3} \mathcal{A}_{nm} V_m(E)$$

(43)

where $V_n(E) = \Lambda_n(E)$, for $n = 1, 2$ and $V_3(E) = V_E$ are the free-bound coupling constants. Assuming these coupling constants to be real, we have $\Lambda_n(E) = \sqrt{\Gamma_f/\pi} \sqrt{g_n}$ and $V_E = \sqrt{\Gamma_f/\pi}$.

The form of the term $\mathcal{N}_n = \sum_{m=1}^{3} \mathcal{A}_{nm} V_m(E)$ for each $n = 1, 2$ is equivalent to that of the numerator of $S_n(E)$ described in subsection A. We have proved earlier that the numerator of $S_n(E)$ has a zero for a real eigenvalue of $H_{\text{eff}}$. For $n = 3$ we have the term

$$\mathcal{N}_3 = -\frac{\Gamma_f}{2\pi} \left[ (\tilde{E} - \tilde{\delta}_2)^2 + (\tilde{E} - \tilde{\delta}_2) \left\{ \tilde{\delta}_2 - \tilde{\delta}_1 + q_1 g_1 + q_2 g_2 \right\} + q_2 g_2 (\tilde{\delta}_2 - \tilde{\delta}_1) \right]$$

(44)

This expression shows that while the term $\mathcal{N}_3$ will not, in general, vanish for a real eigenvalue of $\tilde{H}_{\text{eff}}$ while the others two terms $\mathcal{N}_1$ and $\mathcal{N}_2$ will do. $\mathcal{N}_3$ will vanish for a real eigenvalue when the commutative condition is fulfilled. This means that for A-type or B-type BIC as discussed earlier, all three terms $\mathcal{N}_n (n = 1, 2, 3)$ in the numerator will lead to Fano-like structures with a minimum and spike-like maximum, and as the energy will approach towards the minimum the spike will become narrower as in PA absorption spectrum discussed earlier.
Ideally speaking, exactly at BIC there will be no outgoing scattered waves. The reason is obvious - a bound state with infinite lifetime can not give rise to any outgoing wave. So, to detect a signature of BIC via scattering resonances, the BIC should have a small but finite width meaning the eigenvalue should have small imaginary part. The above analysis implies that, when the system parameters are tuned closed to a BIC, the first two terms $N_1$ and $N_2$ that describe the contributions from the two excited bound states will cause Fano-like structure in the $T$-matrix element. Further, when the commutativity condition is fulfilled or nearly fulfilled, A-type or B-type BIC will show up as prominent Fano-like resonances since all three terms in the numerator of Eq. (43) will contribute to the resonance structures. Thus, BIC in cold atoms can be utilized for narrowing magnetic or optical Feshbach resonances or enhancing the lifetime of the resonances. Thus, creating a BIC in cold atoms with lasers, it is possible to manipulate resonant interactions between the atoms.

E. Efficient production of Feshbach molecules using BIC

Here we discuss how BIC can help in efficient production of Feshbach molecules [41] by stimulated radio-frequency spectroscopy. Note that, for $g_1 >> 1$ and $g_2 >> 1$, the amplitude coefficient of $| b_c \rangle$ in B-type BIC is much greater than those of the two excited bound states. This means that when the two stimulated linewidths $\Gamma_1$ and $\Gamma_2$ are much greater than the Feshbach resonance linewidth $\Gamma_f$, by tuning the two detuning parameters to fulfill the BIC condition $\delta_1 = \delta_2 = q(\Gamma_1 + \Gamma_2 - \Gamma_f)$, one can prepare a B-type BIC with large probability amplitude for the closed channel bound state, which then can be converted into a Feshbach molecule by stimulated radio-frequency spectroscopy. The efficiency of the commonly used method of magnetic field sweep for conversion of pairs of bosonic atoms into Feshbach molecules can not usually go beyond 30%. In contrast, the efficiency of BIC-assisted Feshbach molecule formation can be close to unity. For experimental realization of BIC-assisted Feshbach molecule formation, one can use ultracold Na atoms in the parameter regime of the experiment by Inouye et al. [28] and Xu et al. [32].

It is thus possible to suppress the atom loss in magnetic Feshbach resonance (MFR) in a Bose-Einstein condensates by creating BIC with two lasers. This loss occurs primarily due to the disintegration of quasi-bound states into non-condensate atoms that can escape from the trap. To account for the loss, van Abeelen and Verhaar [30] have introduced a “local” lifetime of quasibound state $| \chi \rangle$ due to its exchange coupling to the incoming open channel at an intermediate separation. For
sodium condensate, this coupling occurs at $r \leq 24$ and the local lifetime $\tau_0 = \frac{1}{\gamma_0} = 1.4\mu s$ [30], where $\gamma_0$ is the width due to the coupling. By choosing the bound states $|b_1\rangle$ and $|b_2\rangle$ having outer turning points near $24 a_0$ and making the bound-bound laser couplings $\Omega_1$ and $\Omega_2$ greater than $\gamma_0$, one can expect to suppress the atom loss to some extent. But, substantial suppression of atom loss will result when the collision energy is tuned closed to the energy of a BIC. As we have analyzed earlier, scattering $T$-matrix element shows a minimum when energy becomes equal to the energy of one of the two bound states in continuum. Since the width $\gamma_0$ is given by the energy derivative of the scattering phase shift at the energy of quasi-bound state [42], in the context of our model $\gamma_0$ will correspond to the energy derivative of the phase shift at the minimum point. Thus, our model provides $\gamma_0 \simeq 0$ and so atom loss in magnetic Feshbach resonances of Bose-Einstein condensates can be largely suppressed. Experimental realization of the effect of the suppression of atoms loss in MFR in sodium BEC or in ultracold sodium gas is possible. Because, photoassociation of sodium atoms into relatively shorter-ranged (outer turning points near $r \sim 24a_0$) bound states in $1g$ potential have been experimentally demonstrated [43–45] and used to create light force in PA [46] and to manipulate higher partial-wave interactions [47] via optical optical Feshbach resonance (OFR) [48].

MFR induced Atom loss in BEC is more severe partly due to bosonic stimulation unlike that in degenerate Fermi gases. Feshbach molecular dimers formed of fermionic atoms are found to be more stable [49, 50] due to Pauli blocking. We therefore predict that the formation of fermionic Feshbach molecules by stimulated radio-frequency spectroscopy using BIC will be quite efficient.

F. Two bound states coupled to the continuum

In our model we have so far considered three bound states coupled to the continuum, with one being quasibound state embedded in the ground-state continuum and the two others being excited molecular states. Naturally, question arises as to what happens to the BIC if coupling to one of the bound states is turned off. Let us first consider that one of the lasers, say $L_2$ is absent, that is $g_2 = 0$. Then the effective Hamiltonian reduces to a $2 \times 2$ matrix with second row and second column of the matrix being removed. Writing the resulting $2 \times 2$ effective Hamiltonian in the form $A_1 + iB_1$, the matrix $B_1$ has one eigenvalue equal to zero and the other one equal to $-(\hbar \Gamma_f / 2)(g_1 + 1)$. Taking $E_c \simeq 0$, the condition for the existence of a real eigenvalue is $\tilde{\delta}_1 = q_1 f_1 - q_1$ which is also the condition for the commutativity between $A_1$ and $B_1$. The real eigenvalue is $-q_1$ and the
corresponding eigenvector is
\[
|\psi\rangle_{\text{BIC}} = \frac{1}{\sqrt{\Gamma_1 + \Gamma_f}} \left[ \sqrt{\Gamma_f} | b_1 \rangle - \sqrt{\Gamma_1} | \chi \rangle \right]
\] (45)

Now, for \( E_c \neq 0 \), by measuring the energy from \( E_c \), we recover the standard result for condition of the occurrence of Fano minimum
\[
\frac{E - E_c}{\hbar \Gamma_f / 2} = -q_{1f}
\] (46)
at which population trapping occurs in the state \( |\psi\rangle_{\text{BIC}} \). This should be manifested as a prominent minimum in the scattering cross section or PA rate versus energy plot [21] as in the case of 3 bound states coupled to continuum as discussed above. In fact, a few years back, two experiments [51, 52] have demonstrated minimum in PA loss rate near the resonant value \( B_0 \) of the magnetic field that induces a Feshbach resonance. Though, spectroscopy of photoassociative atom loss or PA loss is an incoherent method, the spectral minimum observed in such incoherent spectrum might be related to a state closely related to \( |\psi\rangle_{\text{BIC}} \). It is expected that in coherent PA spectroscopy or in the measurement of scattering cross sections near \( B_0 \) under the above-mentioned BIC condition, one would be able to observe the discussed minimum and an ultra-narrow resonant structure as a clear signature of the occurrence of BIC. In the experiment of Junker et al. [51], the quasi-bound state \( |\chi\rangle \) is probably weakly coupled (\( \Omega \) being small) to the excited bound state, since the bound-state chosen was relatively long-ranged ensuring stronger free-bound Franck-Condon overlap rather than bound-bound coupling. This means that \( q_{1f} \) should be negative [21] and so the minimum was expected to occur on the positive side of the scattering length, and indeed that was the case in Ref. [51]. In contrast, the experiment by Bauer et al. [52] used a relatively shorter ranged excited bound state and the minimum (though not very prominent) occurred very close to the resonant magnetic field where \( \alpha_s \to \infty \). The minimum position shows slight shift towards negative side of \( \alpha_s \) as the laser is blue-detuned by about 3 MHz (the subplots of Fig.3 of Ref. [52] should be compared). Assuming \( q_{1f} \) to be positive, the BIC condition provides \( \delta_1 = \omega_{b_1} - \omega_{L_1} = -q_{1f}(\Gamma_1 - \Gamma_f) \). Since in experiment of Ref. [52], a narrow Feshbach resonance is used, and relatively strong PA laser is used, \( (\Gamma_1 - \Gamma_f) > 0 \). With blue detuning \( (\omega_{L_1} > \omega_{b_1}) \), the BIC condition will only be fulfilled if \( q_{1f} \) is positive ensuring significant bound-bound coupling. Autler-Townes double-peaked spectral shape will arise when the the real parts of the two eigenvalues are not very far apart. If BIC condition is maintained more precisely, it is expected that one of the peaks would be very narrow and sharp and would correspond to BIC while the other would be relatively broad due to the fact that the other eigenvalue being essentially complex.
We next discuss the situation when the state $| \chi \rangle$ or the magnetic field is absent. Writing the resulting $2 \times 2$ matrix in the form $A_2 + iB_2$, one finds that $B_2$ has a zero eigenvalue and the other eigenvalue is equal to $-(\Gamma_1 + \Gamma_2)$. The effective Hamiltonian has a real eigenvalue when $\delta_1 = \delta_2$. Note that $\delta_1$ and $\delta_2$ refer to the detuning from the light-shifted bound states. The eigenvalue is $\delta = \delta_1 = \delta_2$ and the corresponding eigenvector is

$$| \phi \rangle_{\text{BIC}} = \frac{1}{\sqrt{\Gamma_1 + \Gamma_2}} \left[ \sqrt{\Gamma_2} | b_1 \rangle - \sqrt{\Gamma_1} | b_2 \rangle \right]$$

which is an excited molecular dark state which has been found to be useful to make an optical Feshbach resonance (OFR) more efficient [23].

V. CONCLUSIONS

In conclusions, we have demonstrated theoretically that it is possible to create and manipulate bound states in continuum in atom-atom cold collisions by lasers and a magnetic field, employing currently available techniques of photoassociation and magnetic Feshbach resonance. Our model is composed of 3 bound states interacting with the continuum of scattering states between ground-state cold atoms. Within the framework of effective Hamiltonian methods, we eliminate the continuum and obtain an effective Hamiltonian. The eigenvectors of this effective Hamiltonian with real eigenvalues represent the bound states in continuum. We have provided specific conditions for the occurrence of a BIC in the form of analytical expressions of the relationships between parameters of our model. We have derived photoassociative absorption spectrum and scattering cross sections that can exhibit signatures of a BIC as an ultra-narrow asymmetric peak near a prominent minimum. The minimum occurs exactly at the energy at which BIC occurs. We have analyzed in some detail the possible applications of BIC in controlling cold collisions and efficient production of Feshbach molecules.

The original proposal of von Neuman and Wigner to create a BIC of a particle was through destructive quantum interference of Schrödinger’s waves scattered by a specially designed potential so that there exists no outgoing waves resulting in the trapping of the particle in the continuum. The key mechanism for creating a BIC is the quantum interference which happens not only in scattering of waves but also in different transition pathways in atomic and molecular physics. Bound states in continuum in our model result from the quantum interference in three possible free-bound transition pathways. In case of 2 bound states interacting with the continuum, the effective Hamil-
tonian yields one BIC that occurs at an energy at which Fano minimum takes place. This indicates that BIC in our model does occur due to quantum interference in possible transition pathways. In recent times, utilization and manipulation of quantum interference effects have been essential in demonstrating a number of coherent phenomena, paving the way for emerging quantum technologies. Of late, quantum interference are being considered for manipulating ultracold collisions \cite{53, 54}. The realization of our proposed bound states in continuum in cold collisions will open a new perspective in quantum interference phenomena with cold atoms and molecules.

Appendix A: Derivation of effective Hamiltonian

\[ \hat{V}G = \hat{V}(P + Q)G = \hat{V}PG + \hat{V}QG \]  
\[ QG = QG_0 + \frac{Q}{E - H_0 + i\epsilon} (\hat{V}PG + \hat{V}QG) \]  
which leads to

\[ QG = \frac{1}{E - H_0 - Q\hat{V} + i\epsilon} \left( Q + Q\hat{V}PG \right) \]  

Substituting (A3) in (A1) and Eq. (6), after some algebra, we get

\[ PGP = \frac{1}{E - H_0 - \hat{P}\hat{V}P - \hat{P}\hat{V}Q + \frac{1}{E - H_0 - Q\hat{V}Q + i\epsilon} Q\hat{V}P} \]

which suggests that the effective Hamiltonian is

\[ H_{\text{eff}} = H_0 + PRP \]  

where

\[ R = \hat{V} + \hat{V}Q \frac{1}{E - H_0 - Q\hat{V}Q + i\epsilon} Q\hat{V} \]  

Now, in the subspace of 3 bound states, we need to diagonalize $H_{\text{eff}}$. Using Eqs. (2) and (4), we have

\[ Q\hat{V}Q = 0 \]  
and
\[
\frac{1}{\hat{V}Q} = \frac{1}{E - H_0 - Q\hat{V}Q + i\epsilon}Q\hat{V}
\]

\[
= \sum_{n,n'} \left[ \Delta_{nn'}^{\text{shift}}(E) - i\frac{\Gamma_{nn'}(E)}{2} \right] |b_n\rangle\langle b_{n'}| + \left[ \Delta_f^{\text{shift}}(E) - i\frac{\Gamma_f(E)}{2} \right] |b_c\rangle\langle b_c|
\]

\[
+ \left[ \sum_n \left\{ \Delta_{nf}^{\text{shift}}(E) - i\frac{\Gamma_{nf}(E)}{2} \right\} |n\rangle\langle b_c| + \text{C.c.} \right]
\]

where

\[
\Delta_{nn'}^{\text{shift}}(E) = \mathcal{P} \int dE' \frac{\Lambda_n(E')\Lambda_{n'}^*(E')}{E - E'}
\]

\[
h\Gamma_{nn'}(E) = 2\pi \Lambda_n(E)\Lambda_{n'}^*(E)
\]

\[
\Delta_f^{\text{shift}}(E) = \mathcal{P} \int dE' \frac{|V_{E'}|^2}{E - E'}
\]

\[
h\Gamma_f(E) = 2\pi |V_{E'}|^2
\]

\[
\Delta_{nf}^{\text{shift}}(E) = \mathcal{P} \int dE' \frac{\Lambda_n(E')V_{E'}^*}{E - E'}
\]

\[
h\Gamma_{nf}(E) = 2\pi \Lambda_n(E)V_{E}^*
\]

\(\Gamma_f\) is the Feshbach resonance line width. Using (A6) in (A4) and (A3), one can obtain the effective Hamiltonian of Eq. (7) the matrix elements of which are given by

\[
\langle b_n | H_{eff} | b_{n'} \rangle = (E_n - \hbar\omega_{L_n})\delta_{nn'} + \Delta_{nn'}^{\text{shift}}(E) - i\frac{\hbar\Gamma_{nn'}(E)}{2}
\]

\[
\langle b_c | H_{eff} | b_c \rangle = E_0 + \Delta_f^{\text{shift}}(E) - i\frac{\hbar\Gamma_f(E)}{2}
\]

\[
\langle n | H_{eff} | b_c \rangle = \Delta_{nf}^{\text{shift}}(E) + \hbar\Omega_n - i\frac{\hbar\Gamma_{nf}(E)}{2}
\]

[1] J. von Neuman and E. Wigner, Phys. Z. 30, 465 (1929).
[2] L. Fonda and R. G. Newton, Ann. Phys. (N.Y.) 10, 490 (1960).
[3] F. H. Stillinger and D. R. Herrick, Phys. Rev. A 11, 446 (1975).
[4] H. Friedrich and D. Wintgen, Phys. Rev. A 32, 3231 (1985).
[5] A. G. Smart, Phys. Today 66, 14 (2013).
[6] E. N. Bulgakov et al., JETP Lett. 84, 430 (2006); A. F. Sadreev, E. N. Bulgakov, and I. Rotter, Phys. Rev. B 73, 235342 (2006).
[7] F. Capasso et al., Nature (London) 358, 565 (1992).
[8] N. Moiseyev, Phys. Rev. Lett. 102, 167404 (2009).
[9] Y. Plotnik et al., Phys. Rev. Lett. 107, 183901 (2011).
[10] C. W. Hsu et al., Nature 499, 188 (2013).
[11] A. Lami and N. K. Rahman, Phys. Rev. A 33, 782 (1986).
[12] E. Kyröla, J. Phys. B: At. Mol. Phys. 19, 1437 (1986).
[13] S. L. Haan and G. S. Agarwal, Phys. Rev. A 25, 4592 (1987).
[14] C. M. Bender and S. Boettcher, Phys. Rev. Lett. 80, 5243 (1998).
[15] C. M. Bender, Rep. Prog. Phys. 70, 947 (2007).
[16] K. O. Friedrichs, Commun. Pure Appl. Math. 1, 361 (1948).
[17] U. Fano, Phys. Rev. 124, 1866 (1961).
[18] P. W. Anderson, Phys. Rev. 124, 41 (1961).
[19] A. Mostafazadeh, Phys. Rev. Lett. 102, 220402 (2009).
[20] S. Longhi, Phys. Rev. B 80, 165125 (2009).
[21] B. Deb and G. S. Agarwal, J. Phys. B: At. Mol. Opt. Phys. 42, 215203 (2009).
[22] K. Rzazewski and J. H. Eberly, Phys. Rev. Lett. 47, 408 (1981).
[23] S. Saha, A. Rakshit, D. Chakraborty, A. Pal and B. Deb, Phys. Rev. A 89, 063418 (2014).
[24] J. L. Bohn and P. S. Julienne, Phys. Rev. A 60, 414 (1999).
[25] C. Chin, R. Grimm, P. S. Julienne and E. Tiesinga, Rev. Mod. Phys. 82, 1225 (2010).
[26] For a review on early works on photoassociation, see J. Weiner, V. S. Bagnato, S. Zilio and P. S. Julienne, Rev. Mod. Phys. 71, 1 (1999).
[27] For a review on ultracold photoassociation spectroscopy, see K. M. Jones, E. Tiesinga, P. D. Lett and P. S. Julienne, Rev. Mod. Phys. 78, 483 (2006).
[28] S. Inouye et al., Nature (London) 392, 151 (1998).
[29] J. Stenger et al. Phys. Rev. Lett. 82, 2422 (1999).
[30] F. A. van Abeelen and B. J. Verhaar, Phys. Rev. Lett. 83, 1550 (1999).
[31] C. Samuelis et al., Phys. Rev. A 63, 012710 (2000).
[32] K. Xu et al., Phys. Rev. Lett. 91, 210402 (2003).
[33] T. Mukaiyama, J. R. Abo-Shaeer, K. Xu, J. K. Chin and W. Ketterle Phys. Rev. Lett. 92, 180402 (2004).
[34] A. Marte et al., Phys. Rev. Lett. 89, 283202 (2002).
[35] T. Volz et al., Phys. Rev. A 68, 010702 (2003).
[36] S. Dürr, T. Volz and G. Rempe, Phys. Rev. A 70, 031601(R) (2004).
[37] K. E. Strecker, G. B. Partridge and R. G. Hulet, Phys. Rev. Lett. 91, 080406 (2003).
[38] M. W. Zwierlein et al., Phys. Rev. Lett. 91, 250401 (2003).
[39] K. E. Strecker, G. B. Partridge, A. G. Truscott and R. G. Hulet, Nature (London) 417, 150 (2002).
[40] S. E. Pollack et al., Phys. Rev. Lett. 102, 090402 (2009).
[41] For a review on Feshbach molecules, see T. Köhler, K. Göral and P. S. Julienne, Rev. Mod. Phys. 78, 1311 (2006).
[42] C. J. Joachain, Quantum Collision Theory (North-Holland, New York, 1972).
[43] P. D. Lett et al., Phys. Rev. Lett. 71, 2200 (1993).
[44] P. Ratliff et al. J. Chem. Phys. 101, 2638 (1994).
[45] R. Napolitano, J. Weiner, C. J. Williams and P. S. Julienne, Phys. Rev. Lett. 73, 1352 (1994).
[46] E. Gomez, A. T. Black, L. D. Turner, E. Tiesinga, and P. D. Lett, Phys. Rev. A 75, 013420 (2007).
[47] B. Deb and J. Hazra, Phys. Rev. Lett. 103, 023201 (2009).
[48] P. O. Fedichev, Y. Kagan, G. V. Shlyapnikov, and J. T. M. Walraven, Phys. Rev. Lett. 77, 2913 (1996).
[49] J. Cubizolles, T. Bourdel, S. J. J. M. F. Kokkelmans, G.V. Shlyapnikov, and C. Salomon, Phys. Rev. Lett. 91, 240401 (2003).
[50] D. S. Petrov, C. Salomon, and G.V. Shlyapnikov, Phys. Rev. Lett. 93, 090404 (2004).
[51] M. Junker et al. Phys. Rev. Lett. 101, 060406 (2008).
[52] D. M. Bauer, M. L. C. Vo, G. Rempe and S. Dürr, Nature Phys. 5, 339 (2009).
[53] B. Deb, J. Phys. B: At. Mol. Opt. Phys. 43, 085208 (2010).
[54] H. Wu and J. E. Thomas, Phys. Rev. A 86, 063625 (2012).