Feshbach Resonance without a Closed-Channel Bound State

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The physics of Feshbach resonance is analyzed using an analytic expression for the s-wave scattering phase shift and the scattering length a which we derive within a two-channel tight-binding model. Employing a unified treatment of bound states and resonances in terms of the Jost function, it is shown that, for strong interchannel coupling, Feshbach resonance can occur even when the closed channel does not have a bound state. This may extend the range of ultracold atomic systems that can be manipulated by Feshbach resonance. The dependence of the sign of a on the coupling strength in the unitary limit is elucidated. As a by-product, analytic expressions are derived for the background scattering length, the external magnetic field at which resonance occurs, and the energy shift $\varepsilon - \varepsilon_B$, where ε is the scattering energy and ε_B is the bound-state energy in the closed channel (when there is one).

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Introduction.—Feshbach resonance (FR) enables manipulation of the interactions between ultracold atoms; e.g., it allows a repulsive gas to be transformed into an attractive one and vice versa [1–7], as in a BEC-BCS crossover [8]. The paradigm of FR, as in the low energy collision of two ultracold atoms, involves the coupling of an open channel o and a bound state at energy ε_B in (another) closed channel c, giving rise to resonant variations of the s-wave scattering length a [4]. This resonance occurs when $\varepsilon_B \approx \varepsilon$, where ε is the scattering energy, namely, when the energy of the closed channel bound state is close to the threshold of the open channel. This condition can be experimentally implemented by varying an external parameter, such as a static magnetic field B, so that the bound state energy is swept through resonance. As we show below, this paradigm can be extended to the case where the closed channel does not have a bound state.

FR is usually formulated as a two-channel scattering problem, which establishes the relation between the bare parameters of the scattering problem (electronic potentials, coupling strength, scattering energy, and external fields) and the physically relevant observables (e.g., the scattering length versus external field, $a(B)$, the bound states of the coupled system, etc.). In this context, it is useful to consider a two-channel model that allows the derivation of analytical expressions of these observables in order to elucidate their relation to the bare parameters. Such a model is not intended to analyze a specific system in detail in which the intrachannel potentials and the interchannel coupling have a definite form appropriate for the system under study. Rather, it should be sufficiently general and simple and, at the same time, encode the underlying physics. The basic ingredients of a two-channel s-wave scattering problem designed to analyze a FR include (1) the intrachannel potentials $v_o(r)$ of the open channel and $v_c(r)$ of the closed channel (here r is the distance between the two atoms), (2) the interchannel coupling potential $w(r)$ (for simplicity we take a constant coupling strength τ), and (3) an external tunable parameter controlling the energy difference $v \equiv v_c(r) - v_o(r)$ as $r \to \infty$. Experimentally, v is often tuned by varying an external magnetic field, $v = \alpha B$, where the constant α depends on the specific system. Thus, knowing the value $v = v_0$ for which the system has a FR is equivalent to finding the magnetic field B_0 at which the scattering length is infinite.

Our main objective here is to show that FR can occur even when the closed channel does not have a bound state, or even when the atom-atom potential in this channel is repulsive. The motivation for addressing this question is evident: this will demonstrate that systems for which a transition from an attractive gas of atoms to a repulsive gas are feasible even for systems for which $v_c(r)$ does not support a bound state. Using a simple model, we show that this is indeed the case; it is possible to obtain a FR and a bound state of the coupled-channel system for large enough coupling τ of the closed and open channels, even when there is no bound state in the closed channel. As a by-product, analytic expressions are derived for the basic physical observables related to FR in terms of the parameters of the scattering problem and a unified treatment of bound states and resonances is carried out in terms of the Jost function.

Two-channel scattering problem.—The s-wave two-channel scattering problem between two atoms a distance r can be mapped onto a single-particle scattering problem in the center of mass coordinate system governed by the Schrödinger equation (in abstract form)

$$\begin{pmatrix} H_o & w^\dagger \\ w & H_c \end{pmatrix}\begin{pmatrix} u_o \\ u_c \end{pmatrix} = \varepsilon\begin{pmatrix} u_o \\ u_c \end{pmatrix} = k^2\begin{pmatrix} u_o \\ u_c \end{pmatrix}. \tag{1}$$

$H_o = -(d^2/dr^2) + v_o(r)$ and $H_c = -(d^2/dr^2) + v_c(r)$ are the Hamiltonians (in r space) for the open and closed channels composed of the kinetic energy operator and intrachannel potentials v_o and v_c, and $\varepsilon = \varepsilon_k = k^2$. The open and closed channels are coupled by the potential $w(r)$. The boundary conditions satisfied by the closed and open components of the exact wave function are $u_o(0) = u_c(0) = 0$, $u_c(r)_{r\to\infty} = Ae^{-\kappa r}$ and $u_o(r)_{r\to\infty} = B\sin[kr + \delta(k)]$. Here, $\kappa(\varepsilon_k) > 0$, A and B are energy dependent constants, and $\delta(k)$ is the scattering phase shift. The s-wave scattering length is given by

$$a = -\lim_{k\to 0}\frac{\tan\delta(k)}{k}. \tag{2}$$

In the standard picture of FR, the closed channel, when uncoupled from the open channel, is assumed to have a bound state $|B\rangle$ at energy $\varepsilon_B < v_c(\infty)$ and continuum states $\{|p\rangle\}$ at energies $\{\epsilon_p > v_c(\infty)\}$. The scattering states of H_o are defined as $H_o|k\rangle = \varepsilon|k\rangle = k^2|k\rangle$ [assuming $v_o(\infty) = 0$ for simplicity]. Eliminating $|u_c\rangle$ from the set of coupled equations (1) results in a single equation for $|u_o\rangle$, $[H_o + v_{\rm eff}(\varepsilon)]|u_o\rangle = \varepsilon|u_o\rangle$, with an effective potential $v_{\rm eff}(\varepsilon) = wG_c(\varepsilon)w^\dagger$, where $G_c(\varepsilon) = (\varepsilon - H_c)^{-1}$. The T matrix associated with $v_{\rm eff}(\varepsilon)$ is formally given by $T(\varepsilon) = [1 - G_o(\varepsilon)v_{\rm eff}(\varepsilon)]^{-1}$, and, by definition, $a = -C\lim_{k\to 0}\langle k|T(\varepsilon)|k\rangle$, where $C > 0$ is a kinematic constant.

For example, a particularly simple model takes $v_o(r)$ and $v_c(r)$ to be spherical square wells of range R, while $w(r)$ couples the two channels only at R. Explicitly,

$$\begin{aligned} v_c(r) &= v\Theta(r - R) + (v - \Delta)\Theta(R - r), \\ v_o(r) &= -\Lambda\Theta(R - r), \qquad w(r) = \tau\delta(r - R), \end{aligned} \tag{3}$$

where τ is the coupling strength. Despite being a simple model, an exact solution of the scattering problem requires solving a set of coupled transcendental equations. Its numerical solution (see the Supplemental Material [9]) confirms the analytical results obtained within the tight-binding (TB) model to which we now turn.

Tight-binding model.—Starting from the continuous model, we discretize the radial coordinate, $r \to n$, where $n > 0$ is an integer, and replace $-(d^2/dr^2)$ by a second-order difference operator [10]. In second quantization it translates as a hopping term, $-(\sum_{n\geq 1} a_n^\dagger a_{n+1} + \text{H.c.})$, where a_n and $a_n^\dagger$ are the annihilation and creation operators of the scattered particle on the positive integer grid sites $n > 0$. The potentials are

$$\begin{aligned} v_c(n) &= (v - \Delta)\delta_{n,1} + v\Theta(n - 1), \\ v_o(n) &= -\Lambda\delta_{n,1}, \qquad w(n) = \tau\delta_{n,1}. \end{aligned} \tag{4}$$

After treating the closed and open channels separately, we will solve the coupled-channel scattering problem.

The Hamiltonian of the closed channel is

$$H_c = (v - \Delta)a_1^\dagger a_1 + \sum_{n>1}[va_n^\dagger a_n - (a_n^\dagger a_{n-1} + \text{H.c.})]. \tag{5}$$

If the well depth $\Delta > 0$, the potential is attractive at site $n = 1$. The potential height v for $n > 1$ is experimentally tunable (e.g., via magnetic field). Let f_n be the amplitude of the wave function at site n. For a bound state with binding energy ε_B, $f_n = A_c e^{-\kappa(n-2)}$ $(n > 1)$, with $\kappa > 0$ and A_c is a constant. Therefore, for $n > 1$ (i.e., outside the range of the attractive potential), $f_2 = A$, $f_3 = Ae^{-\kappa}$, and $\varepsilon_B = v - 2\cosh\kappa$). Simple manipulations yield

$$\kappa = \log\Delta > 0 \Rightarrow \Delta \geq 1, \qquad \varepsilon_B = v - \left[\Delta + \frac{1}{\Delta}\right]. \tag{6}$$

Thus, there is a threshold potential depth $\Delta > 1$ for having an s-wave bound state. A similar scenario occurs also in a 3D continuous geometry, in contradistinction to symmetric 1D or 2D potentials, where any attractive potential of whatever strength supports a bound state. In the model treated here, at most one bound state can occur [11]. An artifact of the TB model is that, for a repulsive potential with $\Delta < -1$, the closed channel does have a bound state above the upper band edge [12]. To avoid this, we will restrict the potential depth to $\Delta > -1$. To summarize, for $\Delta > 1$ the closed channel has a bound state, while for $1 > \Delta > 0$, v_c is attractive but there is no bound state. Moreover, for $0 > \Delta > -1$, v_c is repulsive and there is no bound state.

For the open channel we use $b_n^\dagger$ and b_n as creation and annihilation operators. The Hamiltonian is

$$H_o = -\Lambda b_1^\dagger b_1 - \sum_{n\geq 1}(b_{n+1}^\dagger b_n + \text{H.c.}). \tag{7}$$

For $\Lambda > 1$, the open channel has a bound state, for $1 > \Lambda > 0$, v_o is attractive, but there is no bound state, whereas for $0 > \Lambda > -1$, v_o is repulsive and there is no bound state. The wave function on site $n \geq 1$ is $g_n = A_o\sin[k(n - 1) + \delta(k)]$, where A_o is a constant. The continuous spectrum is a band of energies,

$$\varepsilon_k = -2\cos k \Rightarrow -2 \leq \varepsilon_k \leq 2, \tag{8}$$

so that the lowest threshold for propagation is $\varepsilon_{k=0} = -2$.

Now, consider the coupled-channel system. The Hamiltonian is

$$H = H_c + H_o + \tau(a_1^\dagger b_1 + \mathrm{H.c.}). \tag{9}$$

In a scattering scenario, the effective particle approaches the "origin," $n = 0$, in the open channel from right to left at a given energy, $\varepsilon_k = -2\cos k$, and is reflected back (rightward) into the open channel. The reflection amplitude, equivalently the S matrix, is $S = e^{2i\delta(k)}$, where $\delta(k)$ is the s-wave phase shift from which a is computed as in Eq. (2). f_n and g_n are the amplitudes of the wave function on site n for the closed and open channels, respectively [analogous of $u_c(r)$ and $u_o(r)$ in the continuous model]. The "asymptotic" forms of f_n and g_n are

$$f_n = A_c e^{-\kappa n}, \qquad g_n = \sin[k(n-1) + \delta(k)] \quad (n > 1), \tag{10}$$

where κ is related to ε_k as $2\cosh\kappa = v - \varepsilon_k \geq 2$. Thus, the "nonleakage" condition, $v - \varepsilon_k > 2$, guarantees that propagation in the closed channel is evanescent. Unlike Eq. (6), here κ is independent of the depth Δ of v_c.

Solution.—Solving the TB equations we obtain a relatively simple expression for $\tan\delta(k)$, independent of $\mathrm{sgn}(\tau)$. Writing $\tan\delta(k) = N/D$ and $q(v,k) = \sqrt{(v-\varepsilon_k)^2 - 4}$, we find

$$\begin{aligned} &N(k,\tau,v,\Delta,\Lambda) \\ &\quad = \{2\tau^2 + \Lambda[v - \varepsilon_k + q(v,k) - 2\Delta]\}\sin k, \\ &D(k,\tau,v,\Delta,\Lambda) \\ &\quad = q(v,k) + v - 2\Delta + (\tau^2 - 1)\varepsilon_k + \Lambda[(2\Delta - v)\cos k \\ &\qquad - q(v,k)\cos k - \cos 2k - 1]. \end{aligned} \tag{11}$$

Because $N(k,\ldots) = -N(-k,\ldots)$ and $D(k,\ldots) = D(-k,\ldots)$, $\delta(-k) = -\delta(k) + n\pi$ ($n =$ integer). Extracting $\delta(k)$ from $\tan\delta(k)$ requires a reference; in the continuum version, $\delta(\infty) = 0$, but in TB, "∞" refers to $k = \pi$.

Next we find at what potential $v = v_0(\tau,\Delta,\Lambda)$ we arrive at a FR as $k \to 0$. This is equivalent to finding the value of the magnetic field B_0 for which there is a FR and $|a| \to \infty$ (an experimentally relevant challenge). Because $N(0,\ldots) = 0$, a necessary condition on v_0 for achieving $|a| = -\lim_{k\to 0}[|\tan\delta(k)|/k] = \infty$ is $D(0,\tau,v_0,\Delta,\Lambda) = 0$. From Eq. (11) we easily obtain

$$v_0(\tau,\Delta,\Lambda) = \frac{[\Lambda - 1 + \tau^2 + \Delta(1-\Lambda)]^2}{[\Delta(1-\Lambda) + \tau^2](1-\Lambda)}. \tag{12}$$

Equation (11) is also a sufficient condition for $|a| = \infty$ because $D(k,\tau,v_0,\Delta,\Lambda)$ vanishes as k^2 when $k \to 0$. Therefore, when $v = v_0$, the denominator D in Eq. (11) vanishes faster than the numerator $N \propto \sin k$ (see Sec. 3 of the Supplemental Material [9]), and thus, $|a| \to \infty$. Hence, for a given τ, Δ, Λ, one can tune $v \to v_0(\tau,\Delta,\Lambda)$, Eq. (12), in order to achieve a FR [equivalently, $|\tan\delta(0)| = \infty$].

The discussion following Eq. (9) dictates that v_0 must be positive in order to guarantee the nonleakage condition of the closed channel as discussed after Eq. (10). Inspecting the expression (12) for v_0, we see that it is reasonable to constrain $\Lambda < 1$. Under this condition, the open-channel potential is attractive (equivalently, $\Lambda > 0$), but it does not support a bound state ($\Lambda < 1$).

In order to substantiate our main result, we need to understand the relationship between the occurrence of bound states in a coupled-channel system and FRs. A uniform treatment of resonances and bound states of the coupled-channel system is achievable in terms of the Jost function. For $v \neq v_0(\tau,\Delta,\Lambda)$ [Eq. (12)], resonances and/or bound states of the coupled system exist for $\varepsilon \neq -2$. To explore this regime we use the Jost function, defined (for fixed τ, Δ, Λ) as

$$f(k,v) \equiv D(k,\tau,v,\Delta,\Lambda) - iN(k,\tau,v,\Delta,\Lambda). \tag{13}$$

The S matrix is given in terms of the Jost function as $S = e^{2i\delta} = (1 + i\tan\delta)/(1 - i\tan\delta) = f(-k,v)/f(k,v)$. The Jost function in ordinary potential scattering is discussed in textbooks on scattering theory, e.g. Ref. [13], but here it is formulated and exactly calculated for a "nonordinary" scattering problem with an effective energy-dependent potential. Considered as a function of the complex variable $z = k + iq$ ($0 \leq k \leq \pi$, $-\infty < q < \infty$), $f(z,v)$ is well defined on the imaginary z axis, $z = iq$, where it is real. Solving $f(iq,v) = 0$ gives the position $q(v)$ that is a pole of the S matrix on the imaginary axis in the z plane. An s-wave bound state appears as an isolated zero of $f(iq, v < v_0)$, with $q > 0$, whereas an s-wave resonance appears as an isolated zero of $f(iq, v > v_0)$, with $q < 0$. In both cases, the energy equals $-2\cosh q < \varepsilon_0 = -2$ (namely, below the continuum threshold), but, strictly speaking, the resonance energy is located on the second Riemann sheet in the complex energy plane. Finally, a FR is a zero of $f(iq, v_0)$ occurring as $q \to 0$. Thus, a small upward shift of v_c turns a zero-energy bound state at $q = 0^+$ into a zero-energy (Feshbach) resonance at $q = 0^-$.

We are now in a position to derive our main result. Equation (12) shows that, for fixed $0 < \Lambda < 1$, it is possible to modify $\Delta \to \Delta'$ and $\tau \to \tau'$ in such a way that $\tau'^2 = \tau^2 + (\Delta - \Delta')(1 - \Lambda)$, without affecting v_0. We employ this property for the case $\Delta > 1$ (the closed channel has a bound state) and $\Delta' < 1$ (no bound state in the closed channel), or even $-1 < \Delta' < 0$. The equality $v_0(\tau,\Delta,\Lambda) = v_0(\tau',\Delta',\Lambda)$ guarantees that in both cases FR exists as is evident from Fig. 1 and as is explained in the caption. However, only the case $\Delta > 1$ is commensurate with the paradigm of the FR spelled at the introduction, according to which a bound state in the closed channel is responsible for FR.

This somewhat unexpected result is not an artifact of the TB model. In the Supplemental Material [9] we present a formal proof for a continuous model and substantiate it

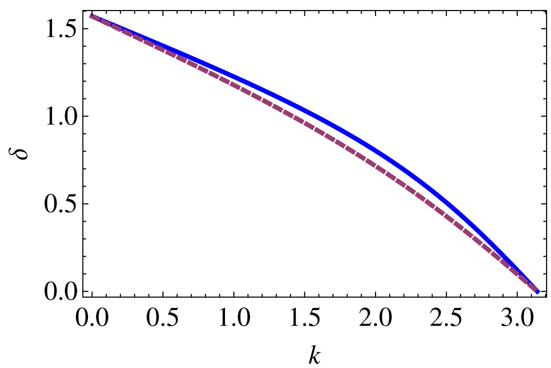

FIG. 1 (color online). Phase shift $\delta(k)$ versus k, Eq. (11). Solid curve: $\tau = 2$, $\Delta = 1.1 > 1$, $\Lambda = 0.2$ (the closed channel has a bound state). Dashed curve: $\tau = 2.227$, $\Delta = -0.1 < 0$, $\Lambda = 0.2$ (the atom-atom potential in the closed channel is repulsive). In both cases $v_0(\tau, \Delta, \Lambda)$ defined in Eq. (12) is equal to 4.264 and $\delta(0) = \pi/2$, implying a FR. The curves are virtually identical for small k because v_0 is determined by the phase shift near $k = 0$.

numerically. To get a simpler (albeit intuitive) physical picture, consider the equation for the open channel $[H_o + v_{\rm eff}(\varepsilon)]\psi_o = \varepsilon\psi_o$, where $v_{\rm eff}(x) = w(x - H_c)^{-1}w^\dagger$. If H_c has only a continuous spectrum starting at $\epsilon_0 > 0$ (i.e., H_c does not have a bound state), then for every $x < 0$ we have $v_{\rm eff}(x) = -w[\sqrt{H_c - x}\sqrt{H_c - x}]^{-1}w^\dagger$ that is a negative definite Hermitian operator. Thus, $v_{\rm eff}(x)$ is a nonlocal attractive potential. By properly tuning the coupling strength τ^2 it is possible to get a zero-energy bound state for $x = \varepsilon = 0^-$. As indicated in the discussion of the Jost function above, a small upward shift of the closed channel potential v_c moves a zero-energy bound state into a zero-energy resonance, i.e., a FR. Summarizing, the physical picture of this new type of FR is as follows: A strong coupling leads to a zero-energy bound state in the equation of the open channel alone (that includes an attractive potential $v_{\rm eff}$). Then, a slight upward shift of the closed channel potential turns this zero-energy bound state into a FR.

Right at FR, $|a| = \infty$. Properties of a unitary gas, where $|a| \approx \infty$, are of great interest in cold atom physics [14]. Direct analysis of Eq. (11) (see Sec. 3 of the Supplemental Material [9]) shows that the unitary gas is attractive or repulsive depending upon the coupling strength τ. Specifically, there exists a threshold τ_0 such that at the FR $a = -\infty(+\infty)$ for $\tau > \tau_0$ $(\tau < \tau_0)$.

Finally, we use our analytic results within the TB model to derive explicit expressions for several important quantities related to FR. The simple expressions for these quantities teach us directly how these physical observables depend on the parameters v, Δ, Λ and τ.

(1) The functional dependence of a on v (that is proportional to the applied magnetic field B) is of utmost importance. Using expression (11) and the definition (2), we immediately obtain

$$a(v) = \frac{2\tau^2 + \Lambda[2(1-\Delta) + v + q(v,0)]}{2[1-\Delta(1-\Lambda) - (\tau^2+\Lambda)] + [v + q(v,0)](1-\Lambda)}. \tag{14}$$

For $v \approx v_0$, $a(v)$ diverges as $a(v) \propto 1/(v - v_0)$, where the proportionality constant is easily calculated.

(2) Another important quantity is the magnetic field B_1 at which the scattering length vanishes, and a changes sign without being singular (recall that $v = \alpha B$). For an atomic gas, whose interaction is given to lowest order by a pseudopotential, this means a change from a repulsive gas to an attractive one (or vice versa). v_1, the solution of $a(v_1) = 0$, is given by, $v_1 = -([\Lambda(1-\Delta) + \tau^2)]^2/\Lambda(\tau^2 - \Delta\Lambda))$. Because of the nonleakage condition, we must have $v_1 > 0$. Hence, $a(v)$ vanishes only when $\Delta\Lambda > \tau^2$.

(3) It is sometimes useful to partition the s-wave scattering length into two terms, $a = a_{\rm bg} + a_{\rm res}$, where $a_{\rm bg}$ is the contribution from the open channel alone and $a_{\rm res}$ is the contribution due to coupling between the closed and open channels. By definition, $a_{\rm bg} = -\lim_{k\to 0}[\tan\gamma(k)/k]$, where $\gamma(k)$ is the phase shift for scattering from the open-channel potential $v_o(n) = -\Lambda\delta_{n,1}$. The result is

$$\tan\gamma(k) = \frac{\Lambda \sin k}{1 - \Lambda \cos k} \Rightarrow a_{\rm bg} = -\frac{\Lambda}{1-\Lambda}. \tag{15}$$

(4) Of special interest is the energy shift $\Delta\varepsilon = \varepsilon_B - \varepsilon_0$ between the bound-state energy of the closed channel (when uncouple) and the scattering energy. $\varepsilon_0 = -2$ at threshold. A FR occurs when $v \to v_0$, as defined in Eq. (12). For $v = v_0$ the closed channel, when uncoupled, has a bound state at energy $\varepsilon_B = v_0 - (\Delta + 1/\Delta)$ [for $\Delta > 1$, see Eq. (6)]. Using this result implies [15]

$$\Delta\varepsilon = \varepsilon_B + 2 = \frac{\tau^2[(1-\Lambda)(\Delta^2-1) + \Delta\tau^2]}{(1-\Lambda)[\Delta(1-\Lambda) + \tau^2]}. \tag{16}$$

For $\Delta > 1$ and $\Lambda < 1$, we have $\Delta\varepsilon > 0$.

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