Quantum Proximity Resonances

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It is well known that at long wavelengths λ an s-wave scatterer can have a scattering cross section σ on the order of λ^2, much larger than its physical size, as measured by the range of its potential. Very interesting phenomena can arise when *two or more* identical scatterers are placed close together, well within one wavelength. We show that, for a pair of identical scatterers, an extremely narrow p-wave "proximity" resonance develops from a broader s-wave resonance of the individual scatterers. A new s-wave resonance of the pair also appears. The relation of these proximity resonances (so called because they appear when the scatterers are close together) to the Thomas and Efimov effects is discussed. [S0031-9007(96)01609-2]

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In quantum scattering theory (or more generally wave scattering) an object "illuminated" by the wave field has two characteristic cross sections. One is the physical size or cross section σ_0 derived from the range r_0 of the perturbation of the medium and the other is an effective cross section σ which is its scattering cross section. Often (and especially in the short wavelength limit) the two sizes are comparable, but σ can be much larger than σ_0. For example, if the scatterer has a long wavelength λ s-wave resonance, where "long" is defined as $\lambda \gg r_0$, then the maximum cross section $\sigma = 4\pi/k^2 = \lambda^2/\pi$ is of the order of the square of the wavelength, which in some cases is thousands of times larger than σ_0.

We might expect something strange to happen when we locate two identical scatterers *inside* each other's effective radius $r_\sigma \equiv \sqrt{\sigma/\pi}$ but *outside* their physical radius r_0. Qualitatively, one scatterer "cannot miss" the other when it scatters the incoming wave. They might pass the wave back and forth for a long time, trapping it in their vicinity. Some examples of this behavior are known, although not perhaps described in just this way. The scattering of light and sound from appropriate objects (see below) are two examples. The present contribution has two purposes: first, to emphasize the generality of the phenomenon, and, second, to show how it arises in quantum scattering, where it apparently has not been described or (as yet) seen.

The phenomenon is easily understood in the case of weak, fixed frequency sound incident on two proximate, small identical air bubbles in water [1,2]. It appears that the phenomenon was first recognized in the bubble scattering context by Tolstoy, where it was called "super-resonance" [1]. For diameters of 10^{-4} M a single bubble is resonant in the audio range [3]. Near the resonance frequency the cross section grows to its s-wave maximum $\sigma_{\max} = 4\pi/k^2$, which corresponds to a disk with a diameter $2\lambda/\pi$, where λ is the wavelength, hundreds of times larger than the diameter of the bubble. For out of phase oscillation one bubble contracts while the other expands, canceling the monopole field, leaving only dipolar radiation from the pair of bubbles, which radiates sound energy much less efficiently. The dipole amplitude goes as kd, where d is the distance between the bubbles, and the radiated power (and resonance width) as k^2d^2.

Another example of this phenomenon can occur in light scattering. Consider two (or more) aligned, resonant molecular dipole light scatterers. These oscillators will be coupled by the radiation field at the incident frequency as well as dipole-dipole interactions and possibly phonons if they are on a surface, etc. This makes the light scattering example more complex than bubbles in water or the quantum scattering considered below, but the essence of the effect is present. A careful self-consistent treatment of the two scatterer problem coupled by the radiation field is beyond the scope of this Letter, but would be an interesting avenue to explore. Some time ago Spruch and Kelsey [4] made very suggestive progress in this regard.

Near resonance the individual cross sections are very large compared to the physical size of the molecules, which can be placed very close together compared to both the cross section and the wavelength. There will be an in-phase symmetric mode, for which the field amplitude is twice that of a single scatterer and the power radiated four times larger; this is twice the power of the two considered incoherently. The radiative lifetime of this mode is half that of a single oscillator, its linewidth twice as large. At a higher frequency there is the antisymmetric mode, which has no dipole moment and is "infrared inactive" in the language of molecular spectroscopy. A small quadrupole (and higher order) field remains with a dramatically reduced radiation rate corresponding to a much narrower resonance than for a single scatterer.

We should expect to see the same phenomenon with other wave equations and scattering theories. Naturally, three or more proximate scatterers will lead to related effects. Here we concentrate on the case of two scatterers. Since the effect goes away as the scatterers are separated, we call the effect *proximity resonance*.

When the scatterer rigidly excludes the wave field, such as hard sphere scattering in quantum mechanics or acoustics, then $\sigma \sim \mathcal{O}(\sigma_0)$ and there will be no proximity resonance. Loosely speaking, in the hard sphere case the scattering is more nearly classical and intuitive because the objects are not placed *inside* their effective diameters. Thus no hint of proximity resonance is contained in the recent literature on the quantum and semiclassical two and three disk scattering problem [5,6].

Proximity resonances are intrinsically a wave phenomenon, far from the semiclassical or ray limit: they require that a single wavelength encompass both scatterers, which are distinct objects. (This however makes application of the *s*-wave multiple scattering theory [7] possible, which we do below). The scatterers necessarily have structure on a scale small compared to a wavelength, violating the usual semiclassical rules.

Consider two small, spherical *s*-wave scatterers placed at fixed distance d apart, with $d > 2r_0$, where $r_0 = \sqrt{\sigma_0/\pi}$. (We treat three dimensional scattering here, but exactly analogous derivations and results exist in two dimensions). The scattering wave function for incoming wave $\psi_0(\vec{r})$ can be written

$$\psi(\vec{r}) = \psi_0(\vec{r}) + \int\int dr'\,dr''\,G_0(\vec{r},\vec{r}\,')T(\vec{r}\,',\vec{r}\,'')\psi_0(\vec{r}\,''), \quad (1)$$

where $T(\vec{r}\,',\vec{r}\,'')$ is the scattering T matrix for the pair of particles at wave number k, and

$$G_0(\vec{r},\vec{r}\,') = \frac{\exp(ik|\vec{r}-\vec{r}\,'|)}{2\pi|\vec{r}-\vec{r}\,'|} \quad (2)$$

is the free Green function. Anywhere outside the scattering centers we may write

$$T(\vec{r}\,',\vec{r}\,'') = \sum_{i,j=1,2} F_{ij}\,\delta(\vec{r}\,'-\vec{r}_i)\delta(\vec{r}\,''-\vec{r}_j). \quad (3)$$

A single scatterer i has its own T matrix and the corresponding wave function is given as

$$\psi(\vec{r}) = \psi_0(\vec{r}) + \int\int dr'\,dr''\,G_0(\vec{r},\vec{r}\,')t(\vec{r}\,',\vec{r}\,'')\psi_0(\vec{r}\,''), \quad (4)$$

with

$$t(\vec{r}\,',\vec{r}\,'') = f\,\delta(\vec{r}\,'-\vec{r}_i)\delta(\vec{r}\,''-\vec{r}_i) \quad (5)$$

leading to the usual asymptotic form

$$\psi(\vec{r}) \to \psi_0(\vec{r}) + f\frac{\exp(ik|\vec{r}-\vec{r}_i|)}{|\vec{r}-\vec{r}_i|} \quad (6)$$

as $|\vec{r}-\vec{r}_i| \to \infty$. The single scattering amplitude f can be written

$$f = f(k) = \frac{\pi}{ik}(e^{2i\delta_0(k)} - 1). \quad (7)$$

The two scatterer amplitude matrix $\mathbf{F}$ is obtained from the one scatterer amplitude f as

$$\mathbf{F} = \begin{pmatrix} 1 & fG_0(\vec{r}_i,\vec{r}_j) \\ fG_0(\vec{r}_i,\vec{r}_j) & 1 \end{pmatrix}^{-1}\begin{pmatrix} f & 0 \\ 0 & f \end{pmatrix} \quad (8)$$

$$\equiv \mathbf{A}^{-1}\mathbf{f}. \quad (9)$$

In the present problem symmetry dictates $F_{11} = F_{22} = \alpha; F_{12} = F_{21} = \beta$. Given that the scattering centers are much closer than a wavelength, we can profitably extract the $s, p, \ldots$ components of $\psi(\vec{r})$ in terms of α and β. We expand the scattered wave about the mean position (taken to be $\vec{r} = 0$) of the pair of scatterers, which lie along the z axis at $\pm d/2$. Using $\psi_0(\vec{r}) = \exp(i\vec{k}\cdot\vec{r})$, we obtain for the diagonal S-matrix elements $S_{l=0,1}$, to order d^2,

$$\frac{i}{2k}(1 - S_0) = \frac{\alpha+\beta}{4\pi}\left(1 - \frac{k_z^2 d^2}{2}\right). \quad (10)$$

$$\frac{3i}{2k}(1 - S_1) = \frac{\alpha-\beta}{4\pi}k_z k d^2. \quad (11)$$

We can parametrize the individual scattering amplitudes f conveniently using the R-matrix formalism [8]; assuming an R-matrix radius a we have

$$f = \frac{\pi}{ik}e^{2ika}\left[\frac{(1+ikR)}{(1-ikR)} - 1\right], \quad (12)$$

where

$$R = R^0(E) + R_{\rm res}(E) = R^0(E) + \frac{\gamma_\nu^2}{(E_\nu - E)}, \quad (13)$$

where E_ν is the single scatterer resonance energy and $R^0(E)$ is the background R matrix. The single scatterer resonance width is $\Gamma = 2k\gamma_\nu^2$.

The "pure resonance" (no background scattering) case leads to simple formulas for the two new resonances which appear in the scattering with both scatterers present. We set $a = 0$ and $R^0(E) = 0$, and look for resonance poles (zeros of $\det \mathbf{A}$) in the complex k plane. We obtain, setting $\det \mathbf{A} = 0$,

$$\frac{E_\nu - k_\pm^2/2 + ik_\pm\gamma_\nu^2}{E_\nu - k_\pm^2/2 - ik_\pm\gamma_\nu^2} = \pm e^{-ik_\pm d}(2ik_\pm d). \quad (14)$$

Writing $k_\pm \equiv k_{r\pm} + ik_{i\pm}$, where $k_{r\pm}$ and $k_{i\pm}$ are real, we find the new resonance energies $E_\pm - i\Gamma_{\nu_\pm}/2 = (k_{r\pm} + ik_{i\pm})^2/2$ with

$$k_{i\pm} \approx -\gamma_\nu^2\left(1 \pm \frac{\sin k_\nu d}{k_\nu d}\right). \quad (15)$$

This gives

$$E_\pm = \frac{k_{r\pm}^2}{2} \approx E_\nu - \left[\pm\frac{\gamma_\nu^2}{d}\cos(k_\nu d)\right]. \quad (16)$$

Approximately,

$$k_{i+} \approx -2\gamma_\nu^2. \tag{17}$$

$$k_{i-} \approx -\gamma_\nu^2 E_\nu d^2/3\,. \tag{18}$$

The imaginary parts of the resonance energies are then

$$\Gamma_+ \approx 4k_\nu \gamma_\nu^2 \tag{19}$$

and

$$\Gamma_- \approx k_\nu^3 \gamma_\nu^2 d^2/3 = \frac{k_\nu^2 d^2}{6}\Gamma\,. \tag{20}$$

We have used the fact that $k_{i\pm}$ is small compared to $k_{r\pm}$, and substituted $\sin k_\nu d/k_\nu d$ for $\sin k_{r\pm} d/k_{r\pm} d$ and $\cos k_\nu d$ for $\cos k_{r\pm} d$; normally this is quite accurate. Note that the "+" resonance is shifted down in energy and has twice the width of the single scatterer. At the complex energy E_+ it is found that the amplitude $\alpha + \beta$ blows up, showing this is an s-wave resonance. The "−" resonance is shifted up in energy and has a much smaller width than the single scatterer. At the complex energy E_- it is found that the amplitude $\alpha - \beta$ blows up, showing this to be a p-wave resonance. The ratio of widths is estimated to be $E_\nu d^2/3$, or about $1/50$ in the case shown below. This is the proximity resonance. Note an interesting fact that the proximity resonance energy is Coulomb repulsive: E_+ increases as d^{-1}, the inverse of the distance between the scatterers.

Figure 1 shows the results of a typical proximity resonance. The cross section as a function of energy is shown for the single scatterer (dashed line), which has a resonance peak at $E_\nu = 0.01$. Shifted to lower energy we find the s-wave two scatterer resonance, which is about twice as broad, as predicted. The very narrow p-wave proximity resonance is shifted an almost equal amount to higher energy. We have assumed the incident wave is along the axis of the two centers; otherwise the p-wave proximity resonance cross section needs to be multiplied by k_z^2/k^2. The proximity resonance is nearly 50 times narrower than the single center resonance. This width decreases as d^2, so if the two centers are physically small and can be placed very close the resonance width can become extremely small.

TABLE I. Predicted and actual real and imaginary parts of resonance energies. $\gamma_\nu^2 = 0.005, \gamma_\nu = 7.07 \times 10^{-4}, E_\nu = 0.01, d = 1$.

	E_-	γ_{ν_-}	E_+	γ_{ν_+}
Predicted	0.01216	1.52×10^{-5}	0.007786	0.00125
Exact	0.01214	1.50×10^{-5}	0.007713	0.00125

Table I shows the results of using the approximate formulas for the resonance position and widths, Eqs. (16), (19), and (20).

If there is a background phase shift the resonances can look very similar or quite different depending on the magnitude and slope of the background phase shift. The proximity resonance can be extremely narrow, broader than the background free case, or even absent. The energy shifts can be reversed. We illustrate with a case of two square wells of depth $V_0 = 21$, range $a = 0.25$, and distance apart $d = 2.2$, providing the background phase shifts to a resonance term $E_\nu = 0.01, \gamma_\nu^2 = 0.005$. The differences with the background free case are dramatic (Fig. 2). Clearly the phenomenology is rich even for two scatterers.

The proximity resonance has some of the flavor of the startling Efimov states, which were discovered more than 25 years ago [9]. Efimov showed that for three particles, with at least two of the three possible pairs interacting "resonantly" at "low" energy, a large or even infinite number of bound states may result. "Resonant" means large scattering length $a_0 \gg r_0$, and low means $kr_0 \ll 2\pi$. These two conditions are similar to those for proximity resonance: $r_\sigma = \sqrt{\sigma/\pi} \gg r_0$, $kd \ll 2\pi$. r_σ plays the role of a_0 above the energy where the scattering length applies. For proximity resonance, one needs a low energy resonance in the individual scatterers, as was the case in the acoustic and light scattering examples cited above. Unlike the Efimov effect, use of the scattering length limit for the s-wave phase shift δ, namely $\delta = -ka_0$, is not sufficient, even if a_0 is large.

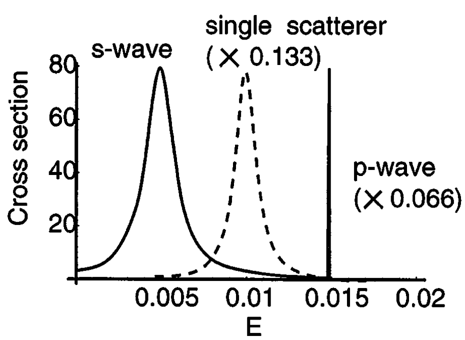

FIG. 1. Cross sections for quantum proximity resonance with no background scattering. See Table I for parameters used.

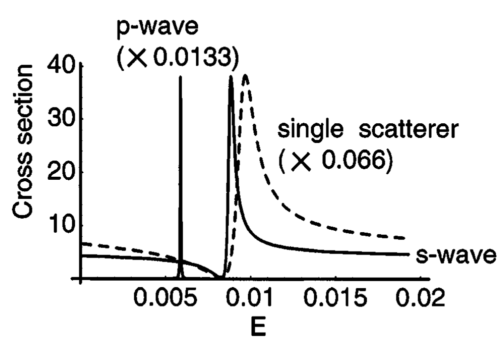

FIG. 2. Cross sections for quantum proximity resonance with background scattering. See text for parameters used.

Efimov generalized his effect to nonidentical particles [10]. Also, Amado and Noble [11] considered different mass ratios, including the "Born-Oppenheimer" case of two heavy and one light particle. This is the case closest to ours. We can think of the fixed scatterers considered here as simply adiabatically slow; however, unlike the Efimov effect we are strictly considering scattering resonances, not bound states.

A related effect was discovered by Thomas [12] even earlier, more than 60 years ago. He showed that the binding energy of three particles interacting by potentials of range r_0 increases without bound as $r_0 \rightarrow 0$. As Adhikari *et al.* made clear [13], the Efimov and Thomas effects are related; Efimov corresponds to $a_0 \rightarrow \infty$ for fixed r_0; Thomas corresponds to $r_0 \rightarrow 0$ for fixed a_0. Proximity resonances fall into a larger class of problems together with the Efimov and Thomas effects for which the "quantum size" is much larger than potential range and distance between the particles, with resulting nonintuitive effects. This Letter is a contribution to understanding this wider class of problems, which we suspect will grow with the addition of other examples.

The conditions for a proximity resonance are rather restrictive for atomic systems, as are the Efimov and Thomas effects. Nonetheless given a low energy resonance it may be possible to see them. Proximity resonances persists in two dimensions, where it is possible to fix two or more atoms on a surface and scatter an electron from them [14]. It is possible that electron or phonon scattering from two or more nearby defects or impurities, near the bottom of a band, may give a three dimensional example in crystal lattices.

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