Quantum proximity resonances

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Abstract

The zero-range potential approximation is used to show that quantum proximity resonances discussed recently by Heller [Phys. Rev. Lett. 77 (1996) 4122] may also occur in the absence of single-scatterer resonances. It is argued that for two identical scatterers a resonant structure appears in the $\Sigma_s$-wave rather than in the $P$-wave partial cross section. © 1997 Elsevier Science B.V.

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In a recent Letter, Heller [1] discussed scattering of a particle on a pair of non-overlapping identical $S$-wave scatterers placed close together. He found that if an individual scatterer gave rise to an $S$-wave resonance characterized by its energy $E_S$ and width $\Gamma_S$, the cross section for scattering on the pair of scatterers exhibited two resonances in a vicinity of $E_S$. One of the resonances had a width comparable with $\Gamma_S$ while the other one was extremely narrow. Heller concluded that both resonances developed from the single-scatterer resonance ($E_S, \Gamma_S$) and designated the broader one "an $S$-wave proximity resonance" and the narrower one "a $P$-wave proximity resonance".

It is a purpose of the present paper to show that quantum proximity resonances may also appear in the absence of single-scatterer resonances and that for two identical scatterers they are $\Sigma_s$-wave rather than $P$-wave resonances. Our argumentation will be based on a zero-range potential model [2,3] and will closely follow works of Subramanian [4], Drukarev and Yurova [5] and Drukarev [3,6] (cf. also Ref. [7]). Despite several simplifying assumptions built into the zero-range potential model, we have found it ideally suited for the purposes of the present work. The main advantage of the model is that it admits an analytical solution to the problem considered.

Consider the scattering of a beam of particles by a pair of identical zero-range $S$-wave scatterers located at a fixed distance $R$ apart at points

$$r_1 = +R/2, \quad r_2 = -R/2$$

(1)

(we choose the origin of a coordinate system in the midpoint of the interval joining the scatterers). Everywhere except the points $r = \mp R/2$, where the scatterers are located, the Schrödinger equation governing the collision process is

$$\left( -\frac{\hbar^2}{2m} \nabla^2 - E \right) \psi(k_i, r) = 0, \quad r \neq \mp R/2,$$

(2)

where $m$ is the mass and $E > 0$ is the energy of the projectile. We seek a solution to Eq. (2) in the form

$$\psi(k_i, r) = \exp(ik \cdot r) + \psi_{\text{out}}(k_i, r).$$

(3)
The first term on the right-hand side of Eq. (3) describes incident particles of momentum $\hbar k_1$, where

$$|k_1| \equiv k = \sqrt{\frac{2mE}{\hbar^2}},$$

while the second one represents scattered particles and satisfies the usual radiation condition at infinity

$$\psi^{\text{out}}(k_1, r) \rightarrow \infty A(k_1, k_1) \frac{\exp(ikr)}{r},$$

with $A(k_1, k_1)$ being the scattering amplitude and $k_1 = kr/r$ denoting the final wave vector of the particle. The function $\psi^{\text{out}}(k_1, r)$ consists of two waves emitted from the points $r = +R/2$ and $r = -R/2$, respectively, each wave being spherically symmetric around its source (S-wave scatterers!). Eq. (2) and the conditions mentioned above are satisfied if we choose

$$\psi^{\text{out}}(k_1, r) = A_1(k_1) \frac{\exp(ikr - R/2)}{|r - R/2|} + A_2(k_1) \frac{\exp(ikr + R/2)}{|r + R/2|}.$$  

The amplitudes $A_1(k_1)$ and $A_2(k_1)$ are determined by the zero-range potential model boundary conditions imposed on the total wave function $\psi(k_1, r)$ at the scatterers [8, 2, 3]

$$\lim_{r \rightarrow \pm R/2} [1 + \kappa |r \mp R/2| + (r \mp R/2) \cdot \nabla] \psi(k_1, r) = 0,$$

where the parameter $\kappa$ is the reciprocal of the S-wave scattering length of an individual scatterer. Substitution of Eqs. (3) and (6) into the conditions (7) yields a system of algebraic equations for $A_1(k_1)$ and $A_2(k_1)$,

$$(ik + \kappa)A_1(k_1) + \exp(ikR)A_2(k_1) = -\exp(ik_1 \cdot R/2),$$

$$\frac{\exp(ikR)}{R} A_1(k_1) + (ik + \kappa)A_2(k_1) = -\exp(-ik_1 \cdot R/2),$$

the solution of which is readily found to be

$$A_1(k_1) = -R \left( \frac{\cos(k_1 \cdot R/2)}{(\kappa R + \cos kR) + i(kR + \sin kR)} + \frac{\sin(k_1 \cdot R/2)}{(\kappa R - \cos kR) + i(kR - \sin kR)} \right),$$

$$A_2(k_1) = -R \left( \frac{\cos(k_1 \cdot R/2)}{(\kappa R + \cos kR) + i(kR + \sin kR)} - \frac{\sin(k_1 \cdot R/2)}{(\kappa R - \cos kR) + i(kR - \sin kR)} \right).$$

To proceed further, we shall take advantage of the symmetry of the problem. At first, we notice that the scattering system possesses the rotational symmetry about the axis joining the scatterers. This implies that the component of the angular momentum of the projectile along this axis is a constant of the motion (its absolute value is denoted as $A$). Moreover, since the scatterers are identical, the scattering system has a center of symmetry (which is the midpoint of the interscatterer axis) and this implies that particle wave's parity is also conserved. It will be profitable to decompose the scattered wave into partial waves appropriate for the symmetry of the problem. Due to the particularly simple form of the interaction chosen, it is easy to recognize which partial waves contribute to $\psi^{\text{out}}(k_1, r)$. Indeed, two identical interfering $S$-waves radiated from the points $r = \pm R/2$ may give rise only to two $S$-partial waves ($\Lambda = 0$), one even ($\psi^{\text{out}}_{S_e}$) and the other odd ($\psi^{\text{out}}_{S_o}$) under reflection at the center $r = 0$: $\psi^{\text{out}}(k_1, r) = \psi^{\text{out}}_{S_e}(k_1, r) + \psi^{\text{out}}_{S_o}(k_1, r),$ where

$$\psi^{\text{out}}_{S_e}(k_1, r) = \frac{1}{2} \left[ A_1(k_1) + A_2(k_1) \right] \times \left( \frac{\exp(ikr - R/2)}{|r - R/2|} + \frac{\exp(ikr + R/2)}{|r + R/2|} \right),$$

$$\psi^{\text{out}}_{S_o}(k_1, r) = \frac{1}{2} \left[ A_1(k_1) - A_2(k_1) \right] \times \left( \frac{\exp(ikr - R/2)}{|r - R/2|} - \frac{\exp(ikr + R/2)}{|r + R/2|} \right).$$

We are now in a position to evaluate scattering amplitudes, phase shifts and cross sections. Making use in Eqs. (13) and (14) of the asymptotic formula
\[
\exp(ik|r = R/2|) \xrightarrow{r \to \infty} \exp(ik \cdot 1/2) \frac{1}{r}
\]
and utilizing Eqs. (5) and (10)-(12), we find
\[
A(k_i, k_f) = A_{\Sigma_+}(k_i, k_f) + A_{\Sigma_-}(k_i, k_f),
\]
where
\[
A_{\Sigma_+}(k_i, k_f) = -2R \frac{\cos(k_i \cdot R/2) \cos(k_f \cdot R/2)}{(\kappa R + \cos kR) + i(kR + \sin kR)},
\]
\[
A_{\Sigma_-}(k_i, k_f) = -2R \frac{\sin(k_i \cdot R/2) \sin(k_f \cdot R/2)}{(\kappa R - \cos kR) + i(kR - \sin kR)}
\]
are scattering amplitudes for the partial waves $$\Sigma_+$$ and $$\Sigma_-$$, respectively. Eqs. (17) and (18) may be rewritten in the form
\[
A_{\Sigma_+}(k_i, k_f) = 4\pi A_{\Sigma_+}(k) \mathcal{Y}_{\Sigma_+}^* (k_f, R)
\]
\[
A_{\Sigma_-}(k_i, k_f) = 4\pi A_{\Sigma_-}(k) \mathcal{Y}_{\Sigma_-}^* (k_f, R)
\]
where the asterisk denotes the complex conjugation, used here only for conformity with the general theory [7] since the functions \{$$\mathcal{Y}_{\Sigma_+}(k, R)$$\} are real (cf. Eq. (23))
\[
A_{\Sigma_+}(k) = \frac{1}{k} \frac{kR + \sin kR}{(\kappa R + \cos kR) + i(kR + \sin kR)}
\]
and
\[
A_{\Sigma_-}(k) = \frac{1}{k} \frac{kR - \sin kR}{(\kappa R - \cos kR) + i(kR - \sin kR)}
\]
are partial scattering amplitudes for the waves $$\Sigma_+$$ and $$\Sigma_-$$, respectively, while
\[
\mathcal{Y}_{\Sigma_+}^*(k, R) = \frac{\cos(k \cdot R/2)}{\sqrt{2\pi}[1 + (1/kR) \sin kR]},
\]
\[
\mathcal{Y}_{\Sigma_-}^*(k, R) = \frac{\sin(k \cdot R/2)}{\sqrt{2\pi}[1 - (1/kR) \sin kR]}
\]
are angular functions appropriate for symmetry of the problem playing the same role in the case discussed here as spherical harmonics do in the theory of scattering from a central field. It is easy to verify by direct integration that the functions \{$$\mathcal{Y}_{\Sigma_+}(k, R)$$\} are orthonormal in the sense of
\[
\int_{4\pi} d\Omega_k \mathcal{Y}_{\Sigma_+}^*(k, R) \mathcal{Y}_{\Sigma_+}(k, R) = \delta_{\pi\pi'}.
\]
In the limit $$R \to 0$$, the functions $$\mathcal{Y}_{\Sigma_+}(k, R)$$ and $$\mathcal{Y}_{\Sigma_-}(k, R)$$ tend to the normalized spherical harmonics $$y_{00}(\angle(k, R))$$ and $$y_{10}(\angle(k, R))$$, respectively [5].

In accord with the general theory [7], the partial scattering amplitudes $$A_{\Sigma_+}(k)$$ and $$A_{\Sigma_-}(k)$$ may be expressed in terms of eigenphase shifts $$\delta_{\Sigma_+}(k)$$ and $$\delta_{\Sigma_-}(k)$$, respectively, which will be useful in examination of possibility of existence of resonances. Making use of the general formula
\[
A(k) = \frac{1}{k} = \frac{1}{\cot \delta(k) - i},
\]
we find from Eqs. (21) and (22)
\[
\cot \delta_{\Sigma_+}(k) = -\frac{\kappa R + \cos kR}{kR + \sin kR},
\]
\[
\cot \delta_{\Sigma_-}(k) = -\frac{\kappa R - \cos kR}{kR - \sin kR}
\]
The total cross section averaged over all possible directions of incidence of the projectile is
\[
\sigma(k) = \frac{1}{4\pi} \int_{4\pi} d\Omega_k \int_{4\pi} d\Omega_k |A(k, k_f)|^2
\]
and may be written as a sum
\[
\sigma(k) = \sigma_{\Sigma_+}(k) + \sigma_{\Sigma_-}(k)
\]
of partial cross sections
\[
\sigma_{\Sigma_+}(k) = \frac{1}{4\pi} \int_{4\pi} d\Omega_k \int_{4\pi} d\Omega_k |A_{\Sigma_+}(k, k_f)|^2,
\]
\[
\sigma_{\Sigma_-}(k) = \frac{1}{4\pi} \int_{4\pi} d\Omega_k \int_{4\pi} d\Omega_k |A_{\Sigma_-}(k, k_f)|^2,
\]
After straightforward integration one obtains (cf. also Refs. [6,7])
\[
\sigma_{\Sigma_+}(k) = \frac{4\pi}{k^2} \frac{(kR + \sin kR)^2}{(\kappa R + \cos kR)^2 + (kR + \sin kR)^2}
\]
Fig. 1. Partial cross sections $\sigma_{\Sigma_+}(k)$, $\sigma_{\Sigma_-}(k)$ and $\sigma_S(k)$ plotted versus wave number $k$ for different values of $\kappa R$ (with $R = 1.0 a_0$): (a) $(-)$ $\sigma_{\Sigma_+}(k)$; $(-\cdots)$ $\sigma_{\Sigma_-}(k)$; $(\cdots)$ $\sigma_S(k)$ for $\kappa R = -0.1$, (b) same as in (a) but for $\kappa R = 0.5$, (c) same as in (a) but for $\kappa R = 0.99$ (the cross section $\sigma_{\Sigma_-}(k)$ has been multiplied by 0.1), (d) same as in (a) but for $\kappa R = 1.1$.

and

$$
\sigma_{\Sigma_+}(k) = \frac{4\pi}{k^2} \frac{(kR - \sin kR)^2}{(kR - \cos kR)^2 + (kR - \sin kR)^2}.
$$

(32)

These formulae are to be compared with a formula for the cross section for a single $S$-wave scatterer

$$
\sigma_S(k) = \frac{4\pi}{k^2 + \kappa^2}
$$

obtained in the zero-range potential model [2,6].

We are now prepared to discuss conditions under which resonances might appear in partial cross sec-
tions $\sigma_S(k)$ and $\sigma_u(k)$. According to general theory \[10\], a resonance occurs at such an energy $E_{res} = \hbar^2 k_{res}^2 / 2m$, at which a partial cross section reaches its maximum value $4\pi / k_{res}^2$ and simultaneously the time-delay of the particle,

$$\Delta t(E_{res}) = 2\hbar \frac{d\delta(k)}{dE} \bigg|_{E=E_{res}} = \frac{2m}{\hbar k_{res}} \frac{d\delta(k)}{dk} \bigg|_{k=k_{res}}, \tag{34}$$

is much longer than the time,

$$\tau_R(E_{res}) = \frac{mR}{\hbar k_{res}}, \tag{35}$$

which a free particle of energy $E_{res}$ needs to travel the distance $R$, i.e.

$$\frac{\Delta t(E_{res})}{\tau_R(E_{res})} = \frac{2}{R} \frac{d\delta(k)}{dk} \bigg|_{k=k_{res}} \gg 1. \tag{36}$$

A glance at Eqs. (31) and (32) shows that in the case discussed in the present paper resonances in the partial waves $\Sigma_S$ and $\Sigma_u$ might occur at energies $E_{\Sigma_S} = \hbar^2 k_{\Sigma_S}^2 / 2m$ and $E_{\Sigma_u} = \hbar^2 k_{\Sigma_u}^2 / 2m$, respectively, such that

$$\cos k_{\Sigma_S}R = -\kappa R, \quad \cos k_{\Sigma_u}R = \kappa R. \tag{37}$$

Differentiating Eq. (26) with respect to $k$ and utilizing Eqs. (36) and (37), one finds relative time-delays of the waves $\Sigma_S$, $\Sigma_u$ and at energies $E_{\Sigma_S}$ and $E_{\Sigma_u}$, respectively,

$$\frac{\Delta t(E_{\Sigma_S})}{\tau_R(E_{\Sigma_S})} = -2 \frac{\sin k_{\Sigma_S}R}{k_{\Sigma_S}R + \sin k_{\Sigma_S}R}, \tag{38}$$

$$\frac{\Delta t(E_{\Sigma_u})}{\tau_R(E_{\Sigma_u})} = 2 \frac{\sin k_{\Sigma_u}R}{k_{\Sigma_u}R - \sin k_{\Sigma_u}R}. \tag{39}$$

Further development requires analysis of Eqs. (38) and (39). Consider at first Eq. (38). It is seen that the expression on its right-hand side is positive for $(2n - 1)\pi < k_{\Sigma_S}R < 2n\pi$, $n = 1, 2, \ldots$, and that in any of these intervals the value of the expression does not exceed unity, which violates condition (36). This implies that within the framework of the model adopted, proximity resonances do not occur in the $\Sigma_S$-wave. Consider now Eq. (39). The function on its right-hand side is positive for $2n\pi < k_{\Sigma_u}R < (2n + 1)\pi$, $n = 0, 1, \ldots$. In those intervals for which $n \geq 1$, the value of the function does not exceed unity and consequently there are no $\Sigma_u$ proximity resonances for $k_{\Sigma_u}R > \pi$. In turn, in the interval $0 < k_{\Sigma_u}R < \pi$, the function considered decreases monotonically from $+\infty$ to 0 and its value in the midpoint $k_{\Sigma_u}R = \pi/2$ is $4/(\pi - 2) \approx 3.50$. This implies that if $k_{\Sigma_u}R$ falls into the first quadrant (i.e. if $\kappa$ and $R$ are such that $1 > \kappa R > 0$), a pronounced single resonant structure appears in the $\Sigma_u$-partial wave cross section $\sigma_{\Sigma_u}(k)$ around the energy $E_{\Sigma_u} = \hbar^2 k_{\Sigma_u}^2 / 2m$, where $k_{\Sigma_u}R = \arccos \kappa R$ (only the principal branch of the arc cosine is chosen). The width of this proximity resonance is $I_{\Sigma_u} = \hbar / \Delta t(E_{\Sigma_u})$. The closer the value of $\kappa R$ to unity, the longer the life-time of this resonance and the narrower and higher the corresponding peak in the partial cross section $\sigma_{\Sigma_u}(k)$. If $k_{\Sigma_u}R$ falls into the second quadrant (i.e. if $\kappa$ and $R$ are such that $0 > \kappa R > -1$), the maximum in the cross section $\sigma_{\Sigma_u}(k)$ flattens and diminishes as $\kappa R \to -1$. Plots of the partial cross sections $\sigma_{\Sigma_u}(k)$ and $\sigma_{\Sigma_u}(k)$ for selected values of $\kappa R$ are shown in Figs. 1a–1d and compared with plots of the single-scatterer cross section $\sigma_S(k)$ given by Eq. (33).

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References