Fano resonances at light scattering by an obstacle

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Introduction and motivation. Light scattering by an obstacle is one of the fundamental problems of electrodynamics, see, e.g., monographs 1, 2. Nowadays interest to this problem increases even more than ever owing to its numerous applications in subwavelength optics, information processing, nanotechnologies and related fields 3. Recent studies of resonant scattering by small particles with weak dissipation rates (see 4, 5, 6 and references therein) have revealed new and unexpected features, namely the inverse hierarchy of optical resonances, a complicated near-field structure, unusual frequency and size dependencies etc., which allow to name such a scattering anomalous. However, despite the highlighted peculiarities, the physical nature of both normal resonant (Rayleigh) and anomalous scattering is the same and may be described briefly as follows. Incident light excites localized electromagnetic modes in a scattering particle (plasmons or polaritons) oscillating with the frequency of the incident wave $\omega$. The corresponding oscillations of polarization of the particle result in an emission of electromagnetic waves with the same frequency $\omega$ which constitute the scattered light. Resonances in this picture correspond to the cases when $\omega$ occurs close to (the real part of) the eigenfrequency of one of the localized modes.

In the present Letter we reveal that this physical picture is analogous to the well-known case of Fano resonances in quantum physics 7. This analogy sheds a new light to the phenomenon. It allows to employ powerful methods developed in the theory of the Fano resonances (such as, e.g., the Feshbach-Fano partitioning theory) to describe the resonant light scattering. It also explains easily certain features of the anomalous scattering and related problems, namely sharp changes in the scattering diagrams (from preferably forward to backward) upon small changes in $\omega$, recently observed in numerical simulations 8 and a typical asymmetric shape of the resonance lines (see Fig. 1) obtained in the present Letter by analysis of the exact Mie solution of the light scattering problem by a spherical particle 1, 2. We also introduce and study an exactly solvable discrete model with nonlocal coupling simulating wave scattering in systems with reduced spatial dimensionality are discussed as examples.

It should be stressed that though the Fano resonances in light scattering have been discussed before, attention has been paid generally to microscopic aspects of inelastic scattering in a simple plane geometry (see, e.g., Ref. 11). In contrast to that, we focus on elastic light scattering by a finite-size particle when diffraction plays a fundamental role in the scattering process. The scattering is accompanied by a two-step transformation: incident plane wave $\rightarrow$ localized electromagnetic modes $\rightarrow$ scattered light. On account of the second step of this transformation (radiative damping) the localized modes have a finite life-time, being actually quasilocalized even at zero dissipation rate. Note however, that as long as the scattering of a continuous wave is concerned, the losses of energy by the quasilocalized modes are exactly compensated by the gain from the incident wave. Then, the amplitude of the modes becomes time-independent.

Another route for the incident light is just to bypass the scatterer, as well as to excite (nonresonantly) localized modes whose eigenfrequencies lie beyond the close vicinity of $\omega$. Interference of the incident and re-emitted light generates a complicated near-field structure and may give rise either to strong enhancement (constructive
interference) or strong suppression (destructive interference) of the electromagnetic field. The analogy to Fano resonances of a quantum particle scattered by a potential with quasidiscrete levels becomes straightforward. The two possible routes for the incident light correspond to the resonant and direct (background) scattering, while the radiative decay of the (quasi)localized modes is identical to tunnelling from the quasidiscrete level.

Light scattering by a small spherical particle. Though the analogy mentioned is pretty general and valid for any particle size and shape, for the sake of simplicity in what follows we consider light scattering by a small spherical particle described by the exact Mie solution [1, 2]. According to the solution for a plane polarized wave propagating along z-axis with vector \( \mathbf{E} \) parallel to x-axis the intensities of waves scattered in a given direction are described by the expressions

\[
S_{||}^{(s)} = I_{||}^{(s)} \cos^2 \varphi; \quad S_{\perp}^{(s)} = I_{\perp}^{(s)} \cos^2 \varphi,
\]

where the subscripts indicate the corresponding polarization (relative to the incident wave), and up to a certain common multiplier

\[
I_{||}^{(s)} \propto \sum_{\ell=1}^{\infty} \frac{2\ell + 1}{\ell(\ell + 1)} \left( a_{\ell} |P_{l}^{(1)}(\cos \theta)\sin \theta - b_{\ell} P_{l}^{(1)}(\cos \theta)\sin \theta|^2 \right),
\]

\[
I_{\perp}^{(s)} \propto \sum_{\ell=1}^{\infty} \frac{2\ell + 1}{\ell(\ell + 1)} \left( a_{\ell} |\sin \theta|^2 - b_{\ell} P_{l}^{(1)}(\cos \theta)\sin \theta|^2 \right),
\]

Here \( \theta \) and \( \varphi \) are the polar and azimuthal angles of the spherical coordinate frame whose center coincides with that of the particle and z-axis with the propagation direction of the incident wave; \( P_{l}^{(1)}(\cos \theta) \) stands for the associated Legendre polynomial, \( P_{l}^{(1)}/(\cos \theta) = dP_{l}^{(1)}(\cos \theta)/d(\cos \theta) \), scattering amplitudes \( a_{\ell} \) and \( b_{\ell} \) may be written in the following form:

\[
a_{\ell} = \frac{F_{l}^{(a)}(q, \epsilon)}{F_{l}^{(a)}(q, \epsilon) + iG_{l}^{(a)}(q, \epsilon)},
\]

and similar for \( b_{\ell} \) with replacement \( F_{l}^{(a)} \rightarrow F_{l}^{(b)}, \ G_{l}^{(a)} \rightarrow F_{l}^{(b)}, \ G_{l}^{(a)}; \) where \( \epsilon(\omega) \) is the relative (with respect to the environment) dielectric permittivity of the particle, \( q = kR, \ k \) stands for the wavenumber of the incident wave in vacuum and \( R \) for the particle radius. As for \( F_{l}^{(a,b)}, \ G_{l}^{(a,b)}, \) they are expressed in terms of the Bessel \([J_{l+1/2}(\zeta)]\) and Neumann \([N_{l+1/2}(\zeta)]\) functions. The corresponding expressions are cumbersome and may be found in Ref. [3]. The partial scattering cross-section \( \sigma_{\text{sca}}^{(l)} \), is connected with \( a_{\ell}, b_{\ell} \):

\[
\sigma_{\text{sca}}^{(l)} = \frac{2\pi}{k^2} (2\ell + 1)(|a_{\ell}|^2 + |b_{\ell}|^2).
\]

We remind briefly results of the analysis of the Mie solution (for more details see, e.g., [4] and references therein). Optical resonances are defined by the condition \( G_{l}^{(a)}(q, \epsilon_{l}) = 0 \). For a small particle \( q \ll 1 \) the condition \( G_{l}^{(a)}(q, \epsilon_{l}) = 0 \), regarded as an equation for \( \epsilon_{l} \), does not have any real solutions, while solutions of the equation \( G_{l}^{(a)}(q, \epsilon_{l}) = 0 \) have the form \( \epsilon_{l} = -(1 + f)/\ell + O(q^{2}) \). Through the dependence \( \epsilon(\omega) \), these solutions define resonant frequencies \( \omega_{r} \) for non-dissipating materials. For weakly dissipating materials the roots of the equation \( G_{l}^{(a)}(q, \epsilon_{l}) = 0 \) have small imaginary parts. In this case the resonant frequencies are equal to the real parts of the corresponding roots. Next, at \( q \ll 1 \) amplitudes \( b_{\ell} \) are small relative to \( a_{\ell} \) and may be dropped. Regarding \( F^{(a)} \), in this limit \( F_{l}^{(a)} = O(q^{2\ell + 1}) \) and it does not vanish anywhere but at the trivial point \( \epsilon = 1 \); as for \( G^{(a)} \) away from the close vicinity of the resonance frequencies it is of order of one. All together that result in sharp optical resonances for \( \sigma_{\text{sca}}^{(l)} \), with a typical symmetric Lorenzian
However, such a profile is not always the case for \( I_{1,1}^{(s)} \).
Let us first discuss the non-dissipative limit (Im \( \epsilon = 0 \)). Considering excitations of non-resonant modes as background scattering and bearing in mind the narrowness of the resonance lines in this case \[1\] we obtain that the corresponding amplitudes \( a_1 \approx a_{10} \), where \( a_0 = O (q^{2+1}) \) is a purely imaginary quantity equal to \(-iqF_{\ell}^{(a)}(q, \epsilon)/G_{\ell}^{(a)}(q, \epsilon)\). Then, the dipole mode (\( \ell = 1 \)) always plays the dominant role in the background scattering. Accordingly, in the vicinity of the dipole resonance the intensity of the dipole scattering always remains large relative to the contribution of the other modes. As a result interference of the resonant scattering with the background gives rise to only small corrections to the resonant mode and the profiles \( I_{1,1}^{(s)}(\epsilon) \) remain Lorentzian.

For higher-order resonances with \( \ell > 1 \), which are also well pronounced in the non-dissipative limit even for a small particle \[4\], the situation is qualitatively different. In this case the resonances scattering arises from the corresponding background, whose amplitude \( a_0 \) is much smaller than that for the background dipole mode \( (a_{10}) \). As \( \epsilon \) approaches \( \epsilon_{\ell} \) the resonant amplitude rapidly increases and becomes much greater than \( a_{10} \), reaching a maximum at \( \epsilon = \epsilon_{\ell} \) and decreasing back to \( a_{10} \) upon further change of \( \epsilon \). Thus, in the vicinity of \( \epsilon_{\ell} \) there are two points (one to the left, the other to the right from \( \epsilon_{\ell} \)) where \( |a_1| = |a_{10}| \). Therefore, in addition to the constructive interference of the resonant mode with the background dipole scattering at \( \epsilon = \epsilon_{\ell} \) we also find annihilation of the two modes at one of the equal-amplitude-points (passing the resonance adds \( \pi \) to the phase of the resonant mode, so only one of the two points satisfies the necessary phase condition for the destructive interference with the background mode). In this case an asymmetric Fano resonance profile is obtained.

To illustrate this reasoning let us consider the vicinity of the quadrupole resonance (\( \ell = 2 \)). Taking \( F_{1,2}^{(a)} \), \( G_{1}^{(a)} \) at \( \omega = \omega_\ell \), employing expansions of the functions in powers of \( \delta \epsilon = \epsilon - \epsilon_{2} \) [we remind that \( G_{2}^{(a)}(\epsilon, \epsilon_{2}) = 0 \)] one obtains the following approximate expressions for \( I^{(s)} \):

\[
I_{1,1}^{(s)} \propto \left| iq^3 \cos \theta + \frac{q^5 \cos 2\theta}{2(q^5 - 12i\delta \epsilon)} \right|^2, \tag{6}
\]
\[
I_{1,1}^{(s)} \propto \left| iq^3 + \frac{q^5 \cos \theta}{2(q^5 - 12i\delta \epsilon)} \right|^2. \tag{7}
\]

There are two characteristic scales in Eqs. (6), (7), describing (i) a sharp resonant lineshape centered at \( \delta \epsilon = 0 \) with width \( \Gamma = q^5/6 \) \[14\] and (ii) full suppression of the scattering which occurs at much greater scale: \( \delta \epsilon_{\perp} = -q^2 \cos 2\theta/24 \cos \theta \) and \( \delta \epsilon_{\parallel} = -q^2 \cos 2\theta/24 \), but still inside the resonance region (\( |\delta \epsilon_{\parallel,\perp}| \ll 1 \)). Note also that there is change of sign of \( \delta \epsilon_{\parallel,\perp} \) with variation of \( \theta \) shifting of the annihilation point from one side of the resonance peak to another.

Finite dissipation and/or increase in \( q \) will broaden the resonances. It results in an overlap of resonance lines of different orders, which eventually may produce very complex profiles. Nevertheless the phenomenon remains qualitatively the same as long as the dissipation is weak. Profiles of forward and backward scattering, calculated for a potassium colloidal nanoparticle immersed in a KCl crystal, are presented in Fig. 4 as an example. The calculations are performed for a realistic dependence \( \epsilon(\omega) \) fitting actual experimental data. Note, that in accordance with Eqs. \( 1 \), \( 7 \) the points of destructive interference for the forward (\( \theta = 0 \)) and backward (\( \theta = \pi \)) scattering lie on different sides of the corresponding resonant peaks \[12\].

Now let us inspect one-dimensional resonant wave scattering in systems with reduced spatial dimensionality. Numerous examples of such systems could be found, e.g., in book \[16\]. Fano resonances exhibited by these systems have exactly the same nature as those discussed above. To make it sure we consider a localized point defect in a simple 1D discrete chain with interaction between the nearest and next-to-nearest neighbor sites (the nonlocal coupling is a fundamental feature of the model). The model is described by the following set of equations (see also Fig. 2):

\[
\begin{align*}
\frac{d\phi_n}{dt} + \sum_{j=-2}^{2} C_n^m \phi_{n+j} &= 0; \quad C_n^m = \omega_0 \delta_{n0} \delta_{m0}; \quad C_n^m = C_m^n, \tag{8}
\end{align*}
\]

where the integer \( n \) labels the spatial sites. All sites of the chain but a defect situated at \( n = 0 \) are identical. Accordingly, \( C_{n\pm 1}^m = 1 \), \( C_{n\pm 2}^m = \gamma \) for \( |n| > 2 \). As for the defect, \( C_{n\pm 1}^m = \mu \), \( C_{n\pm 2}^m = \mu \gamma \) and \( \omega_0 \) stands for the shift of the defect intrinsic frequency with respect to that for the other sites of the chain.

The solvability condition for a linear travelling wave solution \( \phi \sim \exp(i\omega_0 t - iqn) \) in the defect-free region of Eq. \( 5 \) results in the following dispersion relation:

\[
\omega_q = 2(\cos q + \gamma \cos 2q), \tag{9}
\]

where \( q \) is a (quasi)wave vector. To keep the one-to-one correspondence between \( \omega_q \) and \( q \) from the non-trivial range \( 0 \leq q \leq \pi \) we restrict \( |\gamma| \leq 1/4 \).

The defect-free region allows for another type of solutions whose permitted frequencies cover the entire band...
of those for Eq. (1): $-2(1 - \gamma) \leq \omega_q \leq 2(1 + \gamma)$. These solutions are obtained by assigning complex values to $q$ in Eq. (1) $q = \pi \pm ip$; $p \geq 0$ and correspond to exponentially decaying in space localized states.

To study wave scattering by the defect in our model we consider an incident wave with amplitude equals one advancing from the left \[17\]. Then, the corresponding boundary conditions read:

$$
\phi_n = e^{i\omega t} \begin{cases}
    e^{-i\eta n} + \rho_1 e^{i\eta n} + \rho_2 e^{i\mu n}, & n < -2 \\
    \tau_1 e^{-i\eta n} + \tau_2 e^{-i\mu n}, & n > 2,
\end{cases}
$$  \hspace{1cm} (10)

where $\tau_1$ and $\rho_1$, $\tau_2$ and $\rho_2$ are the transmission and reflection amplitudes of the propagating and evanescent waves from both sides of the defect, respectively. The transmission coefficient $T$ is related to $\tau_1$ by the expression $T = |\tau_1|^2$.

The linear problem Eqs. (8)-(10) is exactly solvable, but the solution is extremely cumbersome. It is remarkable, however, that the expression for $\tau_1$ has a structure identical to that of Eq. (11), namely

$$
\tau_1 = \frac{F(\tau_1)}{F(\tau_1) + iG(\tau_1)},
$$  \hspace{1cm} (11)

where $F(\tau_1)$ and $G(\tau_1)$ are real quantities. Eq. (11) is simplified drastically at small $\gamma$, $\mu$ and $\omega_0$ under the additional restriction of weak coupling between the defect and the chain $\mu^2 \ll |\omega_0\gamma|$. In this case

$$
\tau_1 \approx -\frac{\mu^2 + \gamma \delta \omega}{\mu^2 + \gamma \delta \omega - i\delta \omega/2},
$$  \hspace{1cm} (12)

where $\delta \omega = \omega_q - \omega_0$. The corresponding $T(\delta \omega) = 1$ at $\delta \omega = 0$, i.e., when $\omega_q$ coincides with the intrinsic defect frequency and vanishes at $\delta \omega = -\mu^2/\gamma$, cf. the discussed above resonance scattering of light.

To make sure that the obtained properties of the transmission coefficient are related to the resonant excitation of the defect, we calculate $\phi_0$. In the same approximation (small $\gamma$, $\mu$, $\omega_0$ and $\mu^2 \ll |\omega_0\gamma|$) we find:

$$
\phi_0 \approx -\frac{\mu}{\mu^2 + \gamma \delta \omega - i\delta \omega/2}.
$$  \hspace{1cm} (13)

Thus, $|\phi_0|^2$ exhibits a typical sharp Lorentzian profile centered about $\delta \omega \approx -4\gamma\mu^2$.

More extensive analysis of Eqs. (8)-(10) free from the imposed restrictions for $\gamma$, $\mu$, and $\omega_0$ does not add any qualitative difference to the results presented here, except for the fact, that the locations of resonant transmission and reflection may be separated strongly in the frequency space. Note, though the next-to-nearest sites interaction is crucial to the model, its generalization to more extended interactions (provided the coupling constants become smaller with increase in distance between the interacting sites) gives rise just to small quantitative corrections to the model characteristics.

Conclusions. A deep connection between the light scattering by a finite obstacle and Fano resonances in quantum physics is revealed and illustrated by the analysis of the exact Mie solutions and a one-dimension model. The concept developed in the present Letter may be generalized to more complicated problems, e.g., the scattering by a system of particles including coherent backscattering and weak localization phenomena, scattering in waveguides, etc. In each particular system, the specific resonant states are different but all of them act in the same way being described by the similar physics.

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[1] M. Born, and E. Wolf, Principles of Optics, 7th Edition (Cambridge University Press, UK, 1999).
[2] C. F. Bohren, and D. R. Huffman, Absorption and Scattering of Light by Small Particles (Wiley 1998).
[3] W. L. Barnes, A. Dereux, and T. W. Ebbesen, Nature (London) 424, 824 (2003); S. A. Maier et al., Nat. Mater. 2, 229 (2003).
[4] M. I. Tribelsky and B.S. Luk'yanchuk, Phys. Rev. Lett. 97, 263902 (2006).
[5] M. Bashevoy, V. Fedotov, and N. Zheludev, Opt. Express 13, 8372 (2005).
[6] Z. B. Wang, B. S. Luk’yanchuk, M. H. Hong, Y. Lin, and T. C. Chong, Phys. Rev. B 70, 035418 (2004).
[7] U. Fano, Phys. Rev. 124, 1866 (1961).
[8] B. S. Luk’yanchuk, M. I. Tribelsky, Z. B. Wang, Y. Zhou, M. H. Hong, L. P. Shi, and T. C. Chong, Appl. Phys. A (to be published).
[9] S. Flach, V. Fleurov, A. V. Gorbach, A. E. Miroshnichenko, Phys. Rev. Lett. 95, 023901 (2005).
[10] S. F. Mingaleev, A. E. Miroshnichenko, Yu. S. Kivshar, and K. Busch, Phys. Rev. E 74, 046603 (2006).
[11] L. A. Falkovsky and S. Klama, Physica C 264, 1 (1996).
[12] M. I. Tribelsky, Sov. Phys. JETP 58, 534 (1984).
[13] We should stress this is true only for small particles. If a particle is not small the line width $\sigma^{(f)}(\omega)$ may also have a typical asymmetric Fano resonance shape.
[14] The obtained expression for $\Gamma$ coincides with that given by Eq. (8) in Ref. [4] for the line width of the anomalous scattering. Note that there is a misprint in Eq. (8), Ref. [4] (missed factor 2 in the numerator).
[15] A minor shift of the resonance peak with variation in $\theta$ is caused by the mentioned effects of finite $q$ and finite dissipation.
[16] M. J. Ablowitz, B. Prinari, and A. D. Trubatch, Discrete and continuous nonlinear Schrödinger systems (Cambridge Univ. Press, UK, 2004).
[17] The direction of the wave propagation is given by sign of the group velocity $d\omega/dq$ which is positive at $q > 0$ and $\gamma \leq 1/4$, see Eq. (4).