ARTICLE IN PRESS
JID:PLA AID:24599 /SCO Doctopic: Condensed matter [m5G; v1.218; Prn:3/07/2017; 12:15] P.1 (1-6)
Physics Letters A ••• (••••) •••–•••

Contents lists available at ScienceDirect

Physics Letters A

www.elsevier.com/locate/pla

Designing quantum resonant scatterers at subwavelength scale

Jeng Yi Lee [a], Andrey E. Miroshnichenko [b], Ray-Kuang Lee [a,c]

[a] Institute of Photonics Technologies, National Tsing Hua University, Hsinchu 300, Taiwan
[b] Nonlinear Physics Centre, Research School of Physics and Engineering, The Australian National University, Canberra 2601, Australia
[c] Physics Division, National Center for Theoretical Sciences, Hsinchu 300, Taiwan

A R T I C L E I N F O

Article history:
Received 27 May 2017
Accepted 28 June 2017
Available online xxxx
Communicated by A. Eisfeld

Keywords:
Quantum transport
Scattering theory
Quantum dots
S-matrix method in transport

A B S T R A C T

For an isotropic quantum resonant scatterer, such as a quantum dot embedded in host semiconductors, we propose a method to achieve resonant electron scattering by taking physical quantities into account through the second-order expansion. All needed physical information for spherical harmonic channels in anomalous quantum resonant scattering is revealed in a parameter space as the size of quantum scatterer is comparable to the de Broglie wavelength of incoming matter wave. Our results provide the guideline to realize quantum resonant scatterers with state-of-the-art semiconductor heterostructure technology.

1. Introduction

Wave phenomena from different origins share the same principle of superposition, which can be controlled by properly designed structures. In optics, the study on light scattering by subwavelength particles can be traced back to Lord Rayleigh in early developments to explain the colors in the sky [1]. Based on Lorenz–Mie theory, anomalous light scattering in small particles due to the localized surface plasmonic mode is found when the permittivity, ϵ, of a lossless particle at subwavelength scale meets the resonant condition, i.e., $\epsilon = -\epsilon_m (l+1)/l$. Here, ϵ_m corresponds to the permittivity of the surrounding environment, and l denotes the index for spherical harmonics channels ranging from $l = 1, 2, \ldots \infty$ [2,3]. Nowadays, with state-of-the-art nano-structured technologies, having an efficient way to manipulate and design nano-optics is desirable. Due to such a great enhancement in the near-field, lots of potential applications have been demonstrated on light harvesting, sensing, medical treatment and so on [4–10].

Based on the analogies between classical electrodynamics and quantum mechanics, applying concepts from electromagnetic metamaterials to other areas of physics has received considerable attention [11–15]. For barrier-well potentials formed in a core-shell nano-particle embedded in a host semiconductor material, the cloaking as well as invisibility for the electronic transport are revealed by the scattering cancellation method [16–18]. Quantum cloaking can enhance carrier mobility [19] and may be realized in various solid state systems, such as quantum dots and graphenes [20,21].

Even though similar approaches can be applied both to classical electromagnetic and quantum matter waves, the underlying physical interpretations are different. Through the similar mathematical structure between the Helmholtz wave equation and time-independent Schrödinger equation, there exists the correspondence between the permittivity for electric fields in dielectric materials to the effective mass for quantum wavefunction in potentials. Nevertheless, unlike the classical electrodynamics, the index for spherical harmonics channels in quantum waves starts from $l = 0$, which corresponds to the s-wave scattering. Then, the effective mass information (m^*) for a quantum scatterer is totally missing when $l = 0$, if we only apply the first order expansion to meet the resonant condition.

To solve this problem, we can not rely on the conventional Born approximation that only deals with weak scattering interaction [22]. Physically, the results obtained by first approximation indicate that a quantum particle would be intrinsically deflected with a small angled to the original momentum direction. However, in this work, to meet the quantum resonant scattering, a maximized scattering is expected to accompany with a large momentum transfer. To go beyond the Born approximation, we expand the corresponding spherical Bessel and Neumann functions up to the second-order terms, only with which we can include effective mass and potential into the possible implementation for quantum resonant scatterers. By parameterizing system variables, we show

E-mail address: johnnygod2002@hotmail.com (J.Y. Lee).

http://dx.doi.org/10.1016/j.physleta.2017.06.051
0375-9601/© 2017 Published by Elsevier B.V.

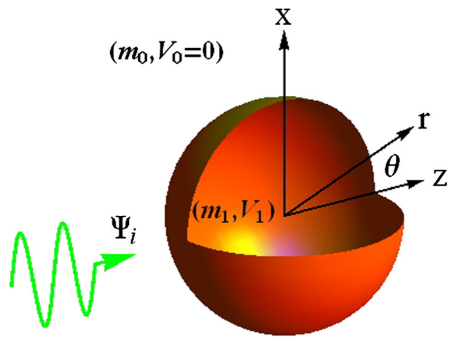

Fig. 1. (Color online.) A schematic view of matter wave scattering by a spherical quantum resonant scatterer. The isotropic and homogeneous effective mass and potential energy inside the scatterer and in the environment are denoted as (m_1, V_1) and $(m_0, V_0 = 0)$, respectively. An incident plane wave for the transport electron, Ψ_i, is assumed to propagate along the z-axis.

a contour plot including all system parameters to satisfy the resonant condition for various quantum angular momentum channels ($l = 0, 1, 2, ..$). A remarkable agreement is also shown in the comparison of our analytical results to the full numerical calculations.

This work seeks for opposite extreme limit in elastic scattering process, quantum resonance scattering, since it can make quantum particles scattered to large directions, equivalent to large momentum transfer occurred with some non-negligible probability. Such anomalous quantum scatterers are desirable for a variety of applications, such as the enhancement of thermoelectric power factor by embedding resonant carriers in thermoelectric materials [23–25], the scanning probes for bosonic atom collisions at ultracold temperatures [26,27], and the observation of quantum proximity resonances [28]. A realistic case has been proposed in semiconductor quantum dots, such as $GaAs/Ga_{1-x}Al_xAs$ materials [29]. In general, in the vicinity of a resonance with respect to energy it is not always possible to employ a characteristic Breit–Wigner formula for the scattering cross section [30], as the profile becomes an symmetric one [31].

By applying our result to a quantum scatterer in the shape of a finite-size sphere, such as a quantum dot, with an isotropic and homogeneous effective mass and potential for the electron transport in a host semiconductor, we also propose a set of alloy semiconductor materials to achieve the s-wave resonance. Our approach provides a compact solution to the practical question on how to build a resonant quantum scatterer precisely for various angular momentum channels when the real material properties are taken into consideration.

2. Theory

We start our analysis by studying the scattering properties of a finite-size spherical scatterer of the radius a, which can be considered as a quantum dot, a dopant or a nanoparticle, see Fig. 1. Such quantum scatterer has isotropic and homogeneous effective mass and local potential, denoted as m_1 and V_1, respectively. The environment could be a host semiconductor with its effective mass m_0 and potential V_0. Without loss of generality, the potential in the surrounding environment can be set to zero, i.e., $V_0 = 0$. The incident quantum matter wave of a single transport electron is assumed to be a plane wave propagating along the z direction, which can be described by the effective Schrödinger equation in time-independent form:

$$-\frac{\hbar^2}{2}\vec{\nabla}\cdot[\frac{1}{m^*(\vec{r})}\vec{\nabla}\psi] + [V(\vec{r}) - E]\psi = 0. \tag{1}$$

Here, the spatial wave function ψ, the effective mass m^*, the effective potential V, and the total energy E are denoted for a single electron, respectively. In the following, we also restrict our study to a Hermitian quantum system with real potentials only. In this scenario, the total probability for the wave function of our transport electron is conserved due to only elastic scattering processes involved. To have a real value in the propagation wavenumber, $k_0 = \sqrt{2m_0E}/\hbar$, both the incident energy E and the effective mass in the environment m_0 are taken to be positive.

As we are dealing with a central scattering potential having rotational invariance, the Hamiltonian commutes with L^2 and L_z, where L is the quantum angular momentum operator. Thus, we can use the eigenstate of L^2 to express the wave function in our scattering system. By using these eigenstates, we express the environmental wave function, ψ_{env}, including incident plane wave and scattering wave: $\psi_{env}(r,\theta) = e^{ikr\cos\theta} + \psi_{scat} = \sum_{l=0}^{l=\infty} i^l(2l+1)[j_l(k_0a) + a_l^{scat}h^{(1)}(k_0a)]P_l(\cos\theta)$. Here, l denotes the quantum angular momentum for the corresponding channel, j_l is spherical Bessel function, a_l^{scat} represents scattering coefficient determined by the radiating boundary conditions, $h^{(1)}$ is the first-kind of spherical Hankel function due to its out-going property for scattering matter wave, and $P_l(\cos\theta)$ is the Legendre polynomial. Meanwhile, inside the scatterer, there exists a transmitted wave written as $\psi_{tr}(r,\theta) = \sum_{l=0}^{l=\infty} i^l(2l+1)t_l j_l(k_1r)P_l(\cos\theta)$, where t_l is unknown transmitted coefficient also determined by boundary conditions and k_1 is transmitted wavenumber defined as $\sqrt{2m_1(E - V_1)}/\hbar$. As our quantum scatterer has the azimuthal symmetry with respect to the rotation around the propagation z-axis, the scattering and transmitted matter waves are also ϕ independent, as expected.

With the continuity of wave function at the boundary and the conservation of probability flux along the radial direction, i.e., $\psi_{env}(a,\theta) = \psi_{tr}(a,\theta)$ and $(1/m_0)(\partial\psi_{env}/\partial r)|_{r=a} = (1/m_1)(\partial\psi_{tr}/\partial r)|_{r=a}$, respectively, one can calculate the two unknown complex coefficients: a_l^{scat} and t_l. Moreover, the scattering coefficient a_l^{scat} can be written in a compact form,

$$a_l^{scat} = -\frac{\zeta_l}{\zeta_l + i\eta_l}, \tag{2}$$

where ζ_l and η_l are:

$$\zeta_l = \frac{k_1}{m_1} j_l'(k_1a)j_l(k_0a) - \frac{k_0}{m_0} j_l'(k_0a)j_l(k_1a) \tag{3}$$

and

$$\eta_l = \frac{k_1}{m_1} j_l'(k_1a)y_l(k_0a) - \frac{k_0}{m_0} y_l'(k_0a)j_l(k_1a), \tag{4}$$

with the spherical Neumann function denoted by $y_l(x)$. Furthermore, to quantify the scattering efficiency, an integration over a closed area can be performed by calculating the scattering probability flux $\vec{J}_{scat}$ at the far field zone (that is $r \to \infty$) per unit incident matter current, $|\vec{J}_{in}| = \hbar k_0/m_0$. With this concept, we can define the scattering cross section accordingly [2]:

$$\sigma^{scat} = \frac{\oint \vec{J}_{scat}\cdot\hat{r}da}{|\vec{J}_{in}|} = \frac{4\pi}{k_0^2}\sum_{l=0}^{l=\infty}(2l+1)|a_l^{scat}|^2, \tag{5}$$

and the transport cross section has the following form:

$$\sigma^{tr} = \oint(1-\cos\theta)\frac{d\sigma^{scat}}{d\Omega}d\Omega \tag{6}$$

$$= \frac{4\pi}{k_0^2}\sum_{l=0}^{l=\infty}(2l+1)|a_l^{scat}|^2 \tag{7}$$

$$-\frac{8\pi}{k_0^2}\sum_{l=0}^{l=\infty}(l+1)Re[(a_l^{scat})^* a_{l+1}^{scat}],$$

Please cite this article in press as: J.Y. Lee et al., Designing quantum resonant scatterers at subwavelength scale, Phys. Lett. A (2017), http://dx.doi.org/10.1016/j.physleta.2017.06.051