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Cloaking Core-Shell Nanoparticles from Conducting Electrons in Solids

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ABSTRACT

In this letter, we aim at making nanoparticles embedded in a host semiconductor with a size comparable to electronic wavelengths “invisible” to the electron transport. Inspired by the recent progress made in the optics, and working within the framework of the expansion of partial waves, we demonstrate that the opposite effects imposed by potential barriers and wells of a core-shell nanoparticle on the phase shifts associated with the scattered electron wave could make the scattering cross section of the first two partial waves vanish simultaneously. We show that this is sufficient to cloak the nanoparticle from being detected by electrons with specific energy in the sense that a total scattering cross section smaller than 0.01% of the physical cross section can be obtained and 4 orders of magnitude difference in the total scattering cross section can be presented within an energy range of only 40meV, indicating possible applications of the “electron cloaks” as novel electronic switches and sensors, and in efficient energy harvesting and conversion technologies.

Keywords: Electron cloak, Partial wave method, Transport, Nanoparticle

In the last decade, the successful design and construction of artificial metamaterials with unusual electromagnetic properties [1-4] opened up new venues to manipulate the propagation and scattering of waves in various forms, as illustrated in the development of different schemes for the “ultimate optical illusion” [2] – invisibility, or the “cloaking effect”. On the other hand, as the characteristic length of electronic devices becomes smaller and smaller, the control of ballistic electron transport processes becomes increasingly important, for which artificial scattering centers would serve as an effective gear. In this letter, we seek for a convergence of the two seemingly unrelated paths.

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Two classes of approaches have been proposed so far to designing optical cloaks, namely transformation optics [1-2, 5] and Mie theory-based scattering cross section minimization [4, 11-13]. Transformation optics utilizes the fact that a coordinate transformation in Maxwell equations is equivalent to a mapping between the distributions of material properties in the two coordinate spaces [5]. A natural extension of this method to quantum matter waves has been intensively investigated recently [6-9], but the resulting anisotropic and/or strongly-spatial dependent distribution of effective mass and/or potential makes the cloaking of electrons extremely difficult to be realized in practical scenarios such as in solid state systems. Conduction electrons in a semiconductor have typical energy of few $k_B T$ (tens of meV) and wavelength of 0.1 to 10 nm. The question we would like to address is whether we can use the freedom of design to create scattering centers inside electronic devices that do not scatter conducting electrons of a specific energy range, and if so, how tunable the energy range and the on-off scattering ratio could be. Such possibility allows the realization of novel filtering and switching devices and has potential applications in quantum information storage, processing and communication, and in situations where a strongly energy-dependent electronic scattering is desirable, such as in thermoelectrics [10]. Moreover, if we can combine the “cloaked” scattering centers and the carrier resources [14], i.e. cloak the carrier donating centers in the relevant energy range, we can improve the carrier mobility significantly and design new materials for semiconductor devices such as transistors and diodes where high carrier mobility is desired.

Applying the Mie theory under the assumption that the scatterer size is much smaller than the optical wavelength, Alú *et al.* [4,11-13] proposed that a properly designed cover made of isotropic and homogeneous plasmonic material or metamaterial could drastically reduce the scattering cross section seen by EM waves of a dielectric (or metal) sphere by vanishing the lowest order electric dipolar contribution, and in subsequent publications, they demonstrated the possibility of canceling both electric and magnetic dipolar contribution at the same time for a larger scatterer [12] or achieving “cloaking” at two different frequencies [4], given more degrees of freedom. Along this approach, a generic difficulty

for electron cloaking is that the practical size of nanoparticles is comparable to the wavelength of conducting electrons in solids, thus the contribution of the waves with higher order angular momentum always play a non-negligible role. Here we adopt a parallel approach formulated within the framework of partial wave method [15] for electrons, which is a close analogy to Mie theory for EM waves, and seek for a simple and intuitive solution that sets the scattering cross sections of the first two partial waves simultaneously to zero. We show that such criterion is sufficient to cloak a nanoparticle with practical size from electrons almost perfectly, in the sense that smaller than 0.01% of the physical cross section would be “seen”.

The classical way of predicting the cross section of scattered waves by a finite-range spherically symmetric potential is the partial wave method [16], where the scattered waves are decomposed into a series of partial waves (PWs) with different angular momenta, and the phase shift of each PW with respect to the incoming wave is calculated by solving the radial Schrödinger equation and applying the continuity of both the wave function and the probability flux at the boundary. For an arbitrary spherically symmetric potential, the phase shift of the l th PW, δ_l , is given by [16]

$$\delta_l = \arctan \left(\frac{kj'_l(ka) - \gamma_l j_l(ka)}{kn'_l(ka) - \gamma_l n_l(ka)} \right) \quad (1)$$

where $k = \frac{\sqrt{2m_0 E}}{\hbar}$ is the wavenumber, a is the radius of the range of the potential, outside of which the

potential is zero, j_l and n_l are spherical Bessel functions of the first and second kind, and $\gamma_l = \left. \frac{\Psi'}{\Psi} \right|_{r=a}$

is the logarithmic derivative of the radial wavefunction at the boundary. After obtaining the phase shifts, the total scattering cross section of electrons with specific incident energy can be found via the general relation [16]:

$$\sigma = \frac{4\pi}{k^2} \sum_{l=0}^{\infty} (2l+1) \sin^2 \delta_l \quad (2)$$

In principle, all the PWs contribute to the total cross section. In practice, however, the phase shifts of higher order PWs are small and the summation converges fast. A general rule of thumb [16] is that the summation converges for angular momentum $l > ka$, indicating that only the lowest few PWs need to be taken into account when ka is small. In semiconductors, the carriers that contribute the most to transport usually reside slightly above the bottom of the conduction band (or below the top of the valence band, as holes). As an estimation, a combination of typical values of the parameters, i.e. energy $E = 10 \text{ meV}$, effective mass $m_0 = 1$, radius of the nanoparticle $a = 2 \text{ nm}$, gives $ka \approx 1$. Thus for practical purposes, nearly zero scattering can be achieved by adjusting parameters to make the cross sections of only 0th and 1st order PWs vanish at the same time.

For the scattering cross section of a certain PW to be zero, the phase shift of the PW must be a multiple of π , as can be seen from Eq. (2). For simplicity and practicality, here we only consider uniform potential wells and barriers. The uniform potential wells and barriers play opposite roles in shifting the phase of the PWs [16], as shown in Fig. 1. A potential well tends to “pull in” the PW or give a negative phase shift, while a barrier does the opposite, and both have a stronger effect on the lower order PWs than the higher order ones. It is relatively easy to achieve zero cross section for only one PW even with a single potential well [16], but it is nontrivial to have a few of PWs with zero scattering at the same energy. With a single potential well (barrier), the 0th order PW tends to pick up a more negative (positive) phase shift than the 1st order one, and the depth (height) required to give rise to a phase difference of π between the two is usually so large that the higher order contributions need to be included. Thus it is extremely difficult, if ever possible, to realize the electron cloak with a single uniform potential well (barrier). Here we demonstrate that this end can be achieved by using a core-shell structured nanoparticle, modeled as a two-step potential barrier (well) as shown in Fig. 2(a) and we

show the coexistence (and counter-play) of the barrier and the well is the key.

Suppose we choose the core to be a barrier, with height $V_1 (> E)$, and effective mass m_1 , and the shell to be a well, with depth $|V_2|$ and effective mass m_2 . By solving the radial Schrödinger equation, and matching the boundary conditions that guarantee the continuity of both the wavefunction and the probability flux, the logarithmic derivative at $r = a$ can be solved as

$$\gamma_l = \frac{m_0}{m_2} \frac{\beta^2 j_l(\alpha a_c) n_l'(\beta a_c) j_l'(\beta a) - \frac{m_2}{m_1} \alpha \beta j_l'(\beta a) j_l'(\alpha a_c) n_l(\beta a_c) + \frac{m_2}{m_1} \alpha \beta j_l(\beta a_c) j_l'(\alpha a_c) n_l'(\beta a) - \beta^2 j_l(\alpha a_c) j_l'(\beta a_c) n_l'(\beta a)}{\beta j_l(\alpha a_c) n_l'(\beta a_c) j_l(\beta a) - \frac{m_2}{m_1} \alpha j_l(\beta a) j_l'(\alpha a_c) n_l(\beta a_c) + \frac{m_2}{m_1} \alpha j_l(\beta a_c) j_l'(\alpha a_c) n_l(\beta a) - \beta j_l(\alpha a_c) j_l'(\beta a_c) n_l(\beta a)} \quad (3)$$

where $\alpha = \frac{\sqrt{2m_1(E-V_1)}}{\hbar^2}$ and $\beta = \frac{\sqrt{2m_2(E-V_2)}}{\hbar^2}$ are wavenumbers in the core and shell region respectively, and a_c is the core radius. The detailed derivation is placed in the Online Supplementary Material [17]. Then the scattering cross sections can be calculated using Eqs. (1) and (2). Rather than looking for solutions of a set of multi-variable nonlinear equations, we discuss the possibility of making both phase shifts of the first two PWs 0 or π by only modifying the barrier height and the well depth, while fixing other parameters, as shown in Fig. 2(b) and 2(c), where we plot the combinations of V_1 and V_2 that give both PWs 0 or π phase shifts given $m_1 = m_2 = m_0 = 1$, and $a_c = 0.5a$. In Fig. 2(b), the two curves do not intersect because in this regime, $|V_2|$ is small and V_1 dominates. Given V_2 , a larger V_1 is required for the 1st order PW to maintain zero phase shift than the 0th order PW (because both barriers and wells have a stronger effect on lower order PW), i.e. the solution curve for the 1st PW always shows a larger slope than that for the 0th PW. In Fig. 2(c), the two curves do intersect and we try to explain the existence of the solution (intersection) by a simple and intuitive argument in terms of the phase shifts. Consider the situation when $V_1 = 0$, a deeper well (a larger $|V_2|$) is required for the 1st PW to gain a phase shift of π than the 0th one for the same reason as mentioned above (this may not always be true, since it is possible that certain choice of the effective mass can give a larger initial phase shift to

the 1st PW than the 0th one. In this case, the solution that makes both phase shifts equal to π does not exist, but the one that makes both phase shifts larger multiples of π can be obtained by similar means). Beyond this point, a given increase of the well depth ($|V_2|$) demands a larger increase of V_1 for the 1st order PW than the 0th order one to keep the phase shift π , again resulting in a larger slope of the solution curve. A deeper (larger) “starting point” and a greater slope of the solution curve for the 1st PW guarantee that the two solution curves would cross each other, generating a combination of V_1 and V_2 that vanishes the cross sections of the first two PWs at the same time. Provided different material properties, one can do similar analysis following the above approach. For instance, in Fig. 3(a) we show the resulting scattering cross sections when the parameters are chosen as $m_1 = 0.9$, $m_2 = 2.2$ and $a_c = 0.75a = 1.5nm$. The corresponding solution of the potentials are $V_1 = 0.057eV$ and $V_2 = -0.788eV$. We observe the dip of the scattering rate at the energy $E = 10meV$ as desired, and the residue scattering cross section smaller than 0.01% of the physical cross section comes from the contribution of higher order PWs. More remarkably, 4 orders of magnitude difference in the total scattering cross section is presented within an energy range of only 40meV. In Figs. 3(b) and (c) we show the radial distribution function of the PWs with and without the nanoparticle, and phase shifts of π are observed as expected outside of the nanoparticle, thus the wavefunctions outside of the nanoparticle are essentially indistinguishable from each other, which is the core of this cloaking scheme. In Fig. 4 we show the “stream lines” of the probability flux, depicting how the incident electron waves “go through” the nanoparticle, where the wavefunction is calculated analytically taking into account partial waves with angular momentum up to $l = 4$.

By adjusting other parameters, a wide range of the barrier heights and well depths can be applicable for electron cloaks, for instance as given in Fig. 5(a), where the ratio between the radii of the core and shell is varied, giving a great flexibility in the practical design. Also we show the energy-dependent scattering rates can be tuned to accommodate different applications via tweaking the effective mass of the core and

shell materials. As shown in Fig. 5(b), different scattering-energy dependences can be obtained by changing the effective mass of the core in a reasonable range. A sharply varying scattering would be good for thermoelectrics and electronic switching and sensing devices, while a flat one may be utilized to cloak electrons with a range of incident energies instead of a single one.

While it seems nontrivial to find proper combinations of materials with the “correct” effective masses and band offsets, this cloaking scheme can be easily implemented on 2D electron gas (2DEG) by proper gating as effective “2D nanoparticles”. The formalism and the resulting scattering “width” of an electron cloak on a GaAs 2DEG is given in Online Supplementary Information [17], which itself can be used as a component in novel electronic switching, sensing and filtering devices. Also potential applications of 3D electron cloaks in thermoelectrics will be discussed in another full-length paper [18].

In summary, we present a simple and flexible scheme of designing electron cloaks using core-shell structured nanoparticles. It must be pointed out that our purpose of this letter is to demonstrate the possibility, rather than give a complete account. Thus there are plenty of other possibilities of achieving electron cloaking based on the same concept, such as making both phase shifts larger multiples of π , setting the core as potential well and shell as barrier, and even conceiving of multilayered structures and so forth. Along this approach, we believe practical combination of materials can be selected and experimental realization of the electron cloaks is achievable given the wide range of possibility and flexibility.

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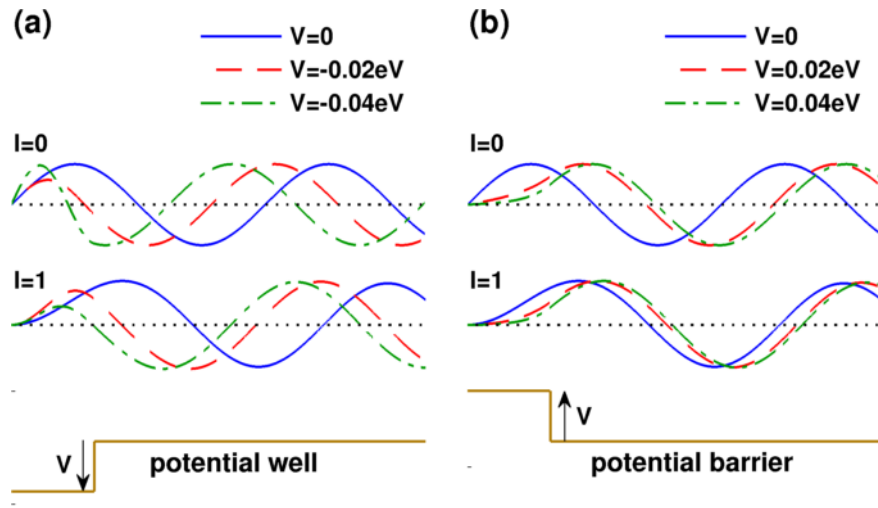


Figure 1. Effects of potential wells and barriers on the PWs. (a) illustrates the “pulling-in” effect of a well on the 0th and 1st order PW; (b) illustrates the “pushing-out” effect of a barrier on the 0th and 1st order PW.

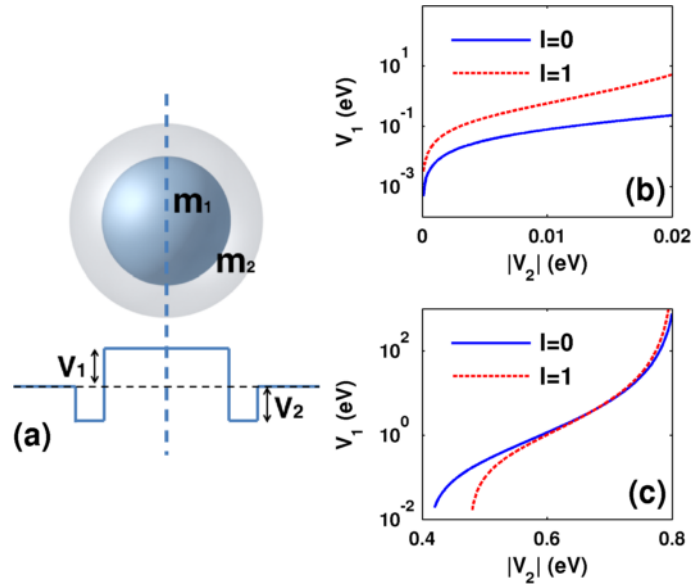


Figure 2 (a) Conceptual illustration of the core-shell nanoparticle. V_1 is the height of the core potential and $|V_2|$ the depth of the shell potential. (b) Combinations of V_1 and V_2 that make the phase shift of the 0^{th} and 1^{st} PW equal to zero respectively. The two curves do not intersect, thus there is no common solution. (c) Combinations of V_1 and V_2 that make the phase shift of the 0^{th} and 1^{st} PW equal to π respectively. The two curves intersect at $V_1 = 3.589 \text{ eV}$ and $V_2 = -0.671 \text{ eV}$. In this case $m_1 = m_2 = m_0 = 1$, and $a = 2 \text{ nm}$, $a_c = 0.5a = 1 \text{ nm}$.

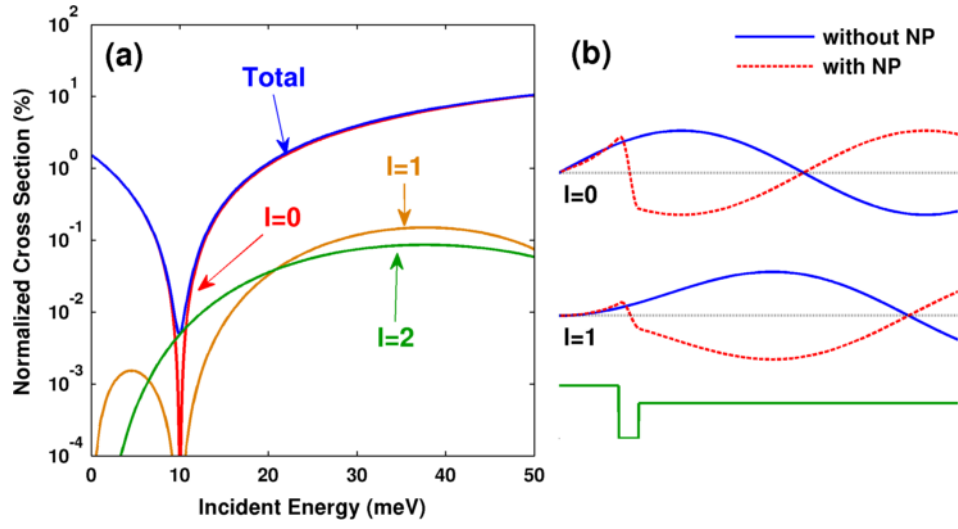


Figure 3 (a) The total scattering cross section and the contributions from the first 3 PWs versus energy. Here the parameters we use are $a = 2nm$, $a_c = 1.5nm$, $m_1 = 0.9$, $m_2 = 2.2$, and correspondingly $V_1 = 0.057eV$ and $V_2 = -0.788eV$. (b) The radial distribution functions of the 0th and 1st PWs with and without the nanoparticle, showing the phase shift of π as expected.

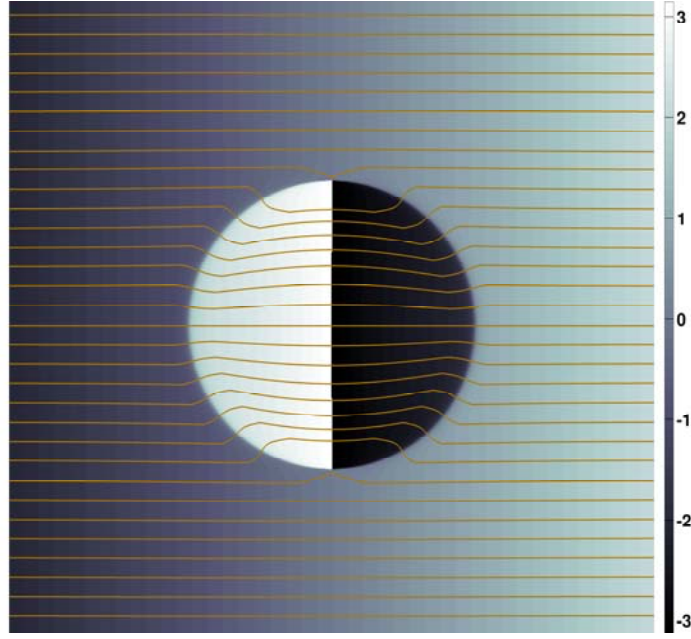


Figure 4 The “stream lines” of the probability flux “going through” the nanoparticle. Background color depicts the phase distribution of the wavefunction. The 2π phase jump at the centerline of the nanoparticle is a numerical artifact. Here the parameters we use are $a = 2nm$, $a_c = 1.5nm$, $m_1 = 0.9$, $m_2 = 2.2$, and correspondingly $V_1 = 0.057eV$ and $V_2 = -0.788eV$.

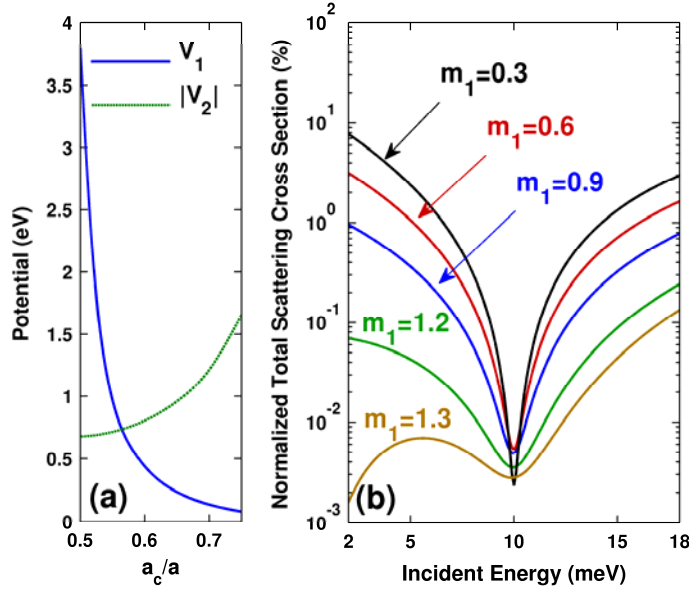


Figure 5 (a) The potentials can be tuned in a wide range by adjusting the ratio between the radii of the core and the shell. Here $m_1 = m_2 = m_0 = 1$ and $a = 2nm$. (b) The energy-dependence of the scattering rates is highly tunable by adjusting, for example, the effective mass of the core m_1 . For this plot $m_2 = 2.2$, $m_0 = 1$ and $a_c = 0.75a = 1.5nm$.