

Entanglement of static and flying qubits in degenerate mesoscopic systems

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The entanglement of flying qubits with static qubits in the solid state is important in the development of quantum computing. It has recently been shown theoretically that the spin-dependent scattering of a propagating electron from a bound electron is sufficient to give full entanglement between the qubits embodied in their respective spins [J. H. Jefferson *et al.*, *Europhys. Lett.* **74**, 764 (2006); D. Gunlycke *et al.*, *J. Phys.: Condens. Matter* **18**, S851 (2006)]. In this paper a generalized, real-space Anderson model is introduced for a quasi-one-dimensional structure consisting of a binding site coupled to ideal leads. Degeneracy of both the binding site and the leads is incorporated to represent, for example, conduction band degeneracy in carbon nanotubes. The model is used to calculate the spin-dependent scattering behavior and resultant static-flying qubit entanglement created by the scattering process. Degeneracy (and more generally, multiplicity) in the binding site gives rise to inelastic scattering processes. In the elastic scattering regime, a degenerate binding site gives rise to antiresonant structures in the transmission spectrum. Additional degeneracy in the leads restricts this effect to the second set of leads, raising the possibility of spin filtration, though this is eliminated in the inelastic scattering regime. Degeneracy in the binding site also gives rise to multiple resonances in transmission that will improve the probability of obtaining entangled pairs relative to the nondegenerate case. This effect is maximized when the components of the degenerate binding site are symmetrically coupled to the leads.

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I. INTRODUCTION

In solid state quantum computation, an attractive candidate for the realization of a qubit is the spin of an electron. The use of an electron spin as a qubit was proposed at an early stage,¹ and there exists a rapidly expanding technology for manipulating single spins in solid state semiconductor structures based on gated quantum wells.^{2–10} The long relaxation and decoherence times^{6–9} of electron spins trapped at quantum dots are encouraging.

Carbon nanotubes are a candidate solid state system for hosting electron spin qubits.^{11–15} The proposed schemes focus on arranging a series of spins confined at quasi-zero-dimensional structures placed along the nanotube. One set of proposals have suggested the use of gate-defined quantum dots.^{16–19} Another set have suggested the use of spin-active endohedral fullerene species, incorporated into “peapod” structures.^{20–22} Examples of such species include Sc@C₈₂, Gd@C₈₂,²³ and N@C₆₀.²⁰ With the recent emergence of single graphite sheet (graphene) experiments, a conceptually related scheme has been proposed in which a strip of graphene acts as the one-dimensional (1D) structure that orders and connects a set of quantum dots, each of which isolates an electron spin qubit.^{24,25}

All of these 1D carbon nanostructure schemes offer the possibility of creating, in a solid state system, a flying qubit. This is a physical realization of a qubit that is moving, allowing information to be transported from one location to another. Proposals for such a flying qubit in the solid state have been rare,²⁶ but would be of great use in implementing a solid state quantum computer. In 1D nanostructures with qubits isolated at quantum dots, the spin of an electron propagating along the host 1D structure could act as a flying

qubit, interacting and exchanging information with the trapped electrons. Following theoretical studies of conduction anomalies in semiconductor nanowires,^{27,28} a scheme has already been proposed for the formation of entangled static-flying qubit pairs.^{29,30}

In the simplest version of this scheme, a shallow potential well is formed in a one-dimensional structure. The well is sufficiently shallow or narrow that it allows only one bound orbital. A single electron is injected into the one-dimensional structure and becomes bound in the well. Subsequent electrons will experience a Coulomb repulsion with the bound electron. It is assumed that this is high enough that the two-electron state associated with the well is only quasibound. Resonant (high probability) transmission will occur for a propagating electron incident on the well with the energy of this quasibound state, but only for the singlet component of the two-electron spin configuration. The exclusion principle dictates that for a well with only one bound orbital, there will be exactly one such Coulomb-mediated quasibound state, and hence at most one, singlet, resonance. For a sufficiently deep and narrow well, a propagating electron will only have a high probability of transmission at energies close to the resonance, and only for the singlet component of the two-electron spin configuration. Hence, conditional on the propagating electron being transmitted, it has a high probability of being in a singlet configuration with the trapped electron. Since the singlet state ($|\uparrow\downarrow\rangle - |\downarrow\uparrow\rangle$) is fully entangled, this scheme projects the state of two electrons into a fully entangled state by the spin-dependent scattering of the propagating electron from the trapped electron. Transmission therefore acts as a singlet spin filter.

In the more general case of a potential well allowing multiple bound orbitals, this scheme can still be implemented if there is a singlet resonance that is well separated in energy

from other resonances. In many cases, the lowest-lying resonance will fulfil these criteria.

In this paper, the possibility of implementing the scheme in a system with multiple bound orbitals is investigated in more depth. Specifically, a generalized real-space Anderson Hamiltonian is used to model a system containing a doubly degenerate binding site, a simple example of a system with multiple bound orbitals. Such a system will have two, typically nondegenerate, bound orbitals. The possibility therefore exists of inelastic scattering of the propagating electron from the bound electron and of multiple resonances. The effects of degeneracy in ideal leads coupling to the binding sites are also investigated. Physical analogs for degeneracy of binding sites and leads include carbon nanotubes or peapods with degenerate conduction channels¹² or semiconductor quantum wires with multiple leads. Analogous for the binding site degeneracy without lead degeneracy include any structure in which two identical quantum dots are coupled to leads. For example, recent work suggests that single-walled carbon nanotube quantum dots may display orbital degeneracy.³¹ The double quantum dot system has received considerable theoretical interest recently.³² It is supposed that a single electron is initially bound in the structure and that a second electron is injected and scatters from it. The spin-dependent scattering behavior of the propagating electron and the resultant entanglement between the flying and the static spin qubit are calculated. The entanglement is entirely dependent on the spin properties of the system. The results of these calculations demonstrate the appearance in a few-electron system of the kind of Fano resonances observed in some transport experiments in carbon nanotubes.³³ The single binding-site scenario previously used in the development of this entanglement scheme is also briefly revisited.^{29,30}

II. ENTANGLEMENT BY SCATTERING IN THE NONDEGENERATE CASE

The subject of this study is the scattering behavior of an electron propagating through a system of degenerate one-dimensional leads and binding sites, from another electron trapped by the binding sites. The effect of the Coulomb interaction at the binding site is of particular interest. This system is modeled using a real-space analog of the Anderson Hamiltonian. The original Anderson Hamiltonian^{34,35} was designed to model a magnetic impurity in a nonmagnetic metal. Real-space analogs describe a binding site coupled to two ideal, discretized leads. A two-electron Coulomb repulsion (U) is included at the binding site. The Hamiltonian can therefore be written as

$$\hat{H} = \hat{H}_R + \hat{H}_L + \hat{H}_c + \hat{H}_I, \quad (1)$$

$$\hat{H}_R = \left[\sum_{n=1}^{\infty} \sum_{\sigma} -t c_{n+1\sigma}^{\dagger} c_{n\sigma} + \varepsilon c_{n\sigma}^{\dagger} c_{n\sigma} \right], \quad (2)$$

and similarly for \hat{H}_L , with the summation over n running from $-\infty$ to -1 . These are the lead Hamiltonians. Here, t and ε are hopping and on-site energies for both of the leads. We

set $\varepsilon=0$ throughout. A propagating electron in these leads will occupy an energy band of the form $E = -2t \cos k$, where k is the electron wave vector. The on-site Hamiltonian for the binding site (\hat{H}_c), which is positioned at $n=0$, is given by

$$\hat{H}_c = \sum_{\sigma} \varepsilon_0 n_{\sigma} + U n_{\uparrow} n_{\downarrow}, \quad (3)$$

$$n_{\sigma} = c_{0\sigma}^{\dagger} c_{0\sigma}. \quad (4)$$

The binding site has on-site single-electron energy ε_0 and Coulomb repulsion U . The interaction Hamiltonian for the leads with the binding site \hat{H}_I is given by

$$\hat{H}_I = t' \sum_{\sigma} (c_{-1\sigma}^{\dagger} c_{0\sigma} + c_{0\sigma}^{\dagger} c_{1\sigma} + \text{H.c.}). \quad (5)$$

The coupling has strength t' .

The approach taken in this study is to use the real-space Anderson Hamiltonian to model a two-electron system. The situation of interest—one electron scattering from another—is incorporated via the boundary conditions. When the two electrons are widely separated, the wave function can be approximated as separable in the coordinates of each electron.

$$\Psi(x_1, x_2) = \begin{cases} (e^{ikx_1} + r e^{-ikx_1}) \psi_b(x_2), & x_1 \ll x_2 \\ p e^{ikx_1} \psi_b(x_2), & x_1 \gg x_2. \end{cases} \quad (6)$$

The propagating electron wave function takes the form of a plane wave that is reflected with amplitude r and transmitted with amplitude p . Probabilities for reflection and transmission are hence $R = |r|^2$ and $P = |p|^2$.

Scattering behavior is calculated separately for the singlet and triplet states, with the antisymmetry principle used to distinguish between the two by symmetrizing (singlet) or antisymmetrizing (triplet) the spatial wave function. The scattering amplitudes r and p are calculated by numerical solution of the Schrödinger equation. A similar approach to calculating scattering behavior was used in a recent study into branched systems.³⁶ Calculated scattering behavior can provide insights into the transport properties of a system, for example, by the use of the Landauer formula.^{37,38}

To explore the behavior of the model and its applications to different physical situations, the scattering behavior is calculated for a range of different parameter values. Only those regimes of interest to entanglement of the static and the flying qubit are explored. First, it is required that the bound electron cannot be ionized by the propagating electron, i.e. that $\varepsilon_b + 2t < -4t$. Second, it is also required that at least one resonance should lie in the single-electron propagating band, as discussed in the Introduction. For example, this gives the requirement for the single channel, single binding site case that $\varepsilon_b - 2t < 2\varepsilon_0 + U < \varepsilon_b + 2t$.

The entanglement between the flying and the static qubit was quantified by calculating the concurrence.³⁹ For a single channel, the concurrence of the qubits can be calculated in the transmission regime of a starting state of antiparallel spins ($|\uparrow\downarrow\rangle$) from the singlet and triplet scattering amplitudes using the formula of Jefferson *et al.* and Ramšak *et al.*,⁴⁰

$$C = \frac{|p_s^2 - p_t^2|}{|p_s|^2 + |p_t|^2}. \quad (7)$$

Here, p_s and p_t are the singlet and triplet transmission amplitudes, respectively.

The scattering and entanglement spectra for the degenerate systems are more easily understood in terms of the results of the nondegenerate, single channel model. In the nonionizing regime and the singlet state, these are approximately equal to those for $\varepsilon_0 \rightarrow -\infty$, $U \rightarrow \infty$, $-2t < \varepsilon_0 + U < 2t$. In this limit, the Schrödinger equation can be solved directly to give the scattering amplitudes as functions of the propagating electron wave vector k , with the triplet state perfectly reflected.

$$p = \frac{i \sin k}{e^{ik} + \nu \left(\frac{\mu}{2} - \nu \cos k \right)}, \quad (8)$$

$$\mu = \frac{\varepsilon_0 + U}{t'}, \quad \nu = \frac{t}{t'}. \quad (9)$$

The transmission spectrum (transmission probability as a function of energy, taken from $-2t$ to $2t$, the whole band of allowed energies for a propagating electron) will have a resonance to $P = |p|^2 = 1$ at energy

$$E = \frac{\varepsilon_0 + U}{1 - \frac{1}{\nu^2}}. \quad (10)$$

Displayed in Fig. 1(a) is the transmission spectrum for one electron scattering from another bound at a binding site in the singlet configuration. As will be the case throughout this paper, the energy axis represents the energy of the propagating electron in units of t . The spectrum presented represents a strongly binding trap site and weak coupling to the leads, with a strong Coulomb interaction. Specifically, $\varepsilon_0 = -10t$, $t' = t/4$, and $U = \varepsilon_0 - t$. These parameters exemplify the regime of interest to the generation of entanglement. A single electron will be tightly bound, but the Coulomb interaction is sufficient that the quasibound two-electron state will be within the propagating electron energy band. The transmission amplitude for singlet scattering matches that given by the formula for $\varepsilon_0 \rightarrow -\infty$ extremely closely and displays the expected resonance to ≈ 1 . Conversely, the transmission amplitude for triplet scattering is close to zero across the whole energy band, again approaching the expected value for $\varepsilon_0 \rightarrow -\infty$.

If we inject an electron into our 1D structure at the resonant energy, the singlet configuration component will almost certainly be transmitted, whereas the triplet configuration will almost certainly not be. If an electron is transmitted, it will be almost maximally entangled with the bound electron. We can quantify this by plotting concurrence as a function of energy using the formulation of Ramšak *et al.* for an antiparallel starting configuration [Fig. 1(b)].

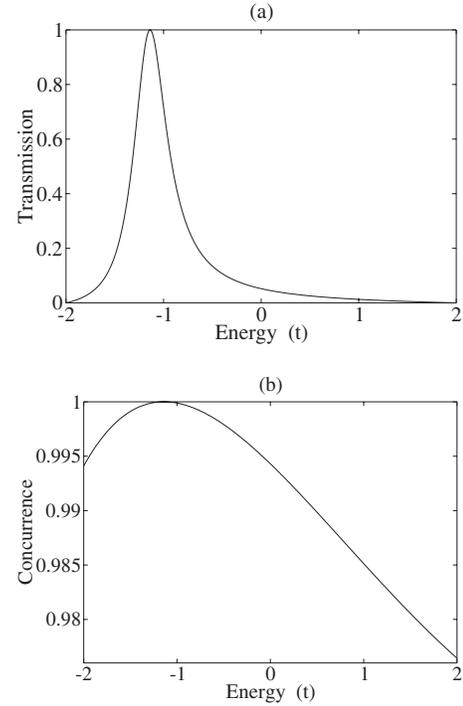


FIG. 1. (a) Singlet scattering. $\varepsilon_0 = -10t$, $t' = t/4$, and $U = \varepsilon_0 + t$. (b) Transmission regime concurrence.

The results in Figs. 1(a) and 1(b) corroborate those obtained by Ramšak *et al.*⁴⁰ using an approximate, analytic model. Concurrence in the transmitted regime peaks around the resonance energy but, encouragingly, remains high across the entire band. The entanglement produced will be more useful when the transmission probability itself is high. Hence, although high entanglement can be found in the transmission regime across the band, it is most useful in the region of the resonance. It is emphasized that the concurrence shown in Fig. 1(b) assumes an antiparallel starting configuration, an even combination of singlet and triplet configurations. Hence, the overall probability of transmission corresponding to that starting configuration will be approximately half that shown in Fig. 1(a).

III. SINGLE-ELECTRON SCATTERING IN DOUBLY DEGENERATE SYSTEMS

Two doubly degenerate systems are investigated in this paper. The first consists of a doubly degenerate binding site (or equivalently two identical nondegenerate binding sites) coupled to ideal leads. One site is connected more strongly to the left lead than the right, and vice versa. The difference is expressed in two different lead-site coupling parameters, t' and t'' . A site-site coupling parameter t_c is also included in the model of this system. The system is shown in Fig. 2.

The Hamiltonian for this system (single-electron terms only) is obtained from Eq. (1) by setting

$$\hat{H}_c = \sum_{\sigma} \left(\sum_l \varepsilon_0 n_{\sigma l} - t_c c_{0\sigma 1}^{\dagger} c_{0\sigma 2} + \text{H.c.} \right) \quad (11)$$

and

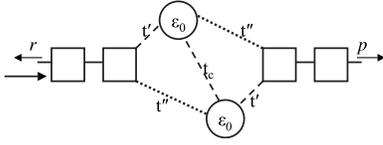


FIG. 2. Scattering from a degenerate binding site.

$$\begin{aligned} \hat{H}_I = & -t' \sum_{\sigma} (c_{-1\sigma}^{\dagger} c_{0\sigma 1} + c_{0\sigma 2}^{\dagger} c_{1\sigma} + \text{H.c.}) \\ & -t'' \sum_{\sigma} (c_{-1\sigma}^{\dagger} c_{0\sigma 2} + c_{0\sigma 1}^{\dagger} c_{1\sigma} + \text{H.c.}). \end{aligned} \quad (12)$$

The two binding sites are indexed $l=1,2$.

The doubly degenerate second system consists of both a degenerate binding site and degenerate leads, effectively giving two coupled one-dimensional structures. The system is shown in Fig. 3.

It is assumed that any electron being injected into the system is initially injected into one set of leads only (the behavior of any other case can be expressed as a linear sum over different injection points). There are now four destinations for the electron. The two degenerate lead-and-binding site structures are indexed with $l=1,2$. The electron can be reflected back the way it came or transmitted via the starting lead set (r_1, p_1) . It can also hop into the second lead set (r_2, p_2) . The designation of the latter two destinations as a reflection and a transmission is somewhat arbitrary and is based around a view of the two channels as lying parallel to each other. The model used here will equally well represent a system in which the second channel lies in a totally different direction to the first. Either way, $r_2=p_2$ by symmetry. The Hamiltonian for this system is

$$\hat{H} = \sum_{l=1,2} \hat{H}_{Rl} + \sum_{l=1,2} \hat{H}_{Ll} + \hat{H}_c + \hat{H}_{coup} + \hat{H}_{int}, \quad (13)$$

where

$$\hat{H}_{Rl} = \left[\sum_{n=1}^{\infty} \sum_{\sigma} -t c_{n+1\sigma}^{\dagger} c_{n\sigma l} + \text{H.c.} + \varepsilon c_{n\sigma l}^{\dagger} c_{n\sigma l} \right], \quad (14)$$

$$\hat{H}_c = \sum_{l=1,2} \sum_{\sigma} \varepsilon_0 n_{\sigma l}, \quad (15)$$

$$\hat{H}_{coup} = -t' \sum_{l=1,2} \sum_{\sigma} (c_{-1\sigma l}^{\dagger} c_{0\sigma l} + c_{0\sigma l}^{\dagger} c_{1\sigma l} + \text{H.c.}), \quad (16)$$

and

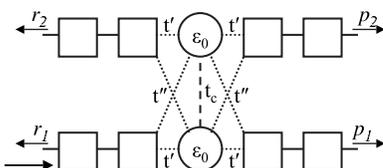


FIG. 3. Scattering in two coupled structures.

$$\begin{aligned} \hat{H}_{int} = & -t'' \sum_{\sigma} (c_{-1\sigma 1}^{\dagger} c_{0\sigma 2} + c_{1\sigma 1}^{\dagger} c_{0\sigma 2} + c_{-1\sigma 2}^{\dagger} c_{0\sigma 1} + c_{1\sigma 2}^{\dagger} c_{0\sigma 1} \\ & + \text{H.c.}) - t_c \sum_{\sigma} (c_{0\sigma 1}^{\dagger} c_{0\sigma 2} + \text{H.c.}). \end{aligned} \quad (17)$$

Here, \hat{H}_c is the Hamiltonian for the two binding sites, \hat{H}_{coup} is the coupling between each binding site and its corresponding leads, and \hat{H}_{int} is the coupling between the two binding sites and lead structures created by the double degeneracy of the binding sites and the leads.

The single-electron scattering behavior of these systems is easy to analyze and provides insight into the more complicated two-electron scattering that generates entanglement. Scattering can be rationalized by taking symmetric and antisymmetric combinations over the two binding sites (in the former system) or over the two lead-and-binding-site structures (in the latter system). The method of decomposing a problem of N coupled channels into N single channel problems by taking appropriate linear combinations of the channels is well established for mesoscopic systems.⁴¹

Following this transformation, the transmission amplitude p for a doubly degenerate binding site can be expressed as $p = p_s - p_a$, where p_s is the amplitude for transmission through a symmetric combination of the binding sites, and p_a is the amplitude for the antisymmetric combination. These amplitudes will have the same form as the single binding-site amplitude noted in the previous section [Eq. (8)] but with the modified parameters: $U=0$ (since this is the single electron case); $\varepsilon_0^s = \varepsilon_0 - t_c$ and $t'_s = t' + t''$ for p_s and $\varepsilon_0^a = \varepsilon_0 + t_c$ and $t'_a = t' - t''$ for p_a . In the regime $-2t < \varepsilon_0 < 2t$, the transmission spectrum will have two resonant peaks. These peaks are found at approximately the energies given by Eq. (10), with the modified parameters $\varepsilon_0 + U \rightarrow \varepsilon_0^s$, $t'^2 \rightarrow t'^2 + t''^2$ and $\varepsilon_0 + U \rightarrow \varepsilon_0^a$, $t' \rightarrow t'_a$, respectively. There is also an antiresonance that occurs when $p_s = p_a$ at

$$E = \varepsilon_0 - \frac{t_a'^2 + t_s'^2}{t_a'^2 - t_s'^2} t_c. \quad (18)$$

If $t' = t''$, the “antisymmetric” resonance and the antiresonance disappear since the site-lead coupling that gives rise to p_a vanishes (and $p_a = 0$). In fact, a single resonance will be found quite generally for an n -fold degenerate binding site, each component of which is coupled equally to both leads and with strength t_c to every other component. The resonance will be found at energy

$$E = \frac{\varepsilon_0 - (n-1)t_c}{1 - n \frac{1}{\nu^2}}. \quad (19)$$

The symmetric and antisymmetric combination of sites in the case of degenerate binding sites and degenerate leads gives two decoupled, nondegenerate structures, each containing a single binding site and set of leads. These are referred to as the “symmetric” and the “antisymmetric” structure. They are identical to the single-binding site Anderson model, with modified parameters as given above for the degenerate binding site structure. The transmission probabilities for the

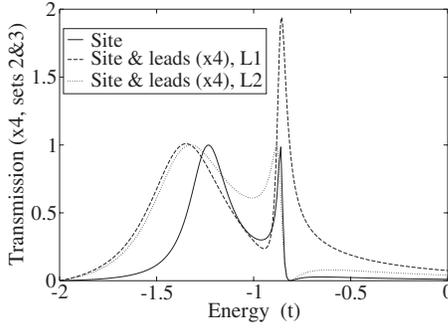


FIG. 4. Single electron transmission spectra for a doubly degenerate binding site and the doubly degenerate site-and-leads structure. $\varepsilon_0=t$, $t'=t/4$, $t_c=0.15t$, and $t''=t/8$. Transmission probabilities for the degenerate-leads structure are multiplied by 4.

doubly degenerate site-and-leads structure are then given by $P_1 = \frac{P_s+P_a}{4}$ and $P_2 = \frac{P_s-P_a}{4}$. The factor 4 is introduced by the multiple branches of the coupled, degenerate system. These probabilities mean that the transmission spectrum of the doubly degenerate site-and-leads structure will have two peaks in transmission through either set of leads, their positions given by Eq. (10) with appropriately modified parameters. Transmission through lead set 2 will also contain an antiresonance, its position again given by Eq. (18).

Transmission spectra for a doubly degenerate binding site and for both lead sets of the doubly degenerate site-and-leads structure are shown in Fig. 4. The parameters used are $\varepsilon_0=t$, $t'=t/4$, $t_c=0.15t$, and $t''=t/8$. Transmission probabilities for the degenerate-leads structure are multiplied by 4 to allow easy comparison with the qualitative form of the degenerate-binding-site structure.

The transmission spectrum for the doubly degenerate binding site structure is qualitatively very similar to that of the second set of leads in the degenerate-leads structure. This similarity extends into the two-electron results. In the following sections, only the results for the second lead set of the degenerate-leads case will therefore be presented. These will be a close match to those for the doubly degenerate binding site.

IV. TWO-ELECTRON SYSTEMS

The scenario of interest in quantum computing is that in which one propagating electron scatters from another, bound electron. To model the interaction between such electrons in degenerate binding sites, two types of term are added to the Hamiltonians discussed in the previous section. The first is an on-site Coulomb repulsion term, Un_1n_1 , for each binding site, as in the nondegenerate Anderson Hamiltonian. The second is an inter-binding-site repulsion term, $Vn_{0\sigma}n_{0\sigma'}$.

Because there are two binding sites in the systems under consideration, there will be two (typically nondegenerate) bound orbitals, one of which will be symmetric with respect to the binding sites, and one of which will be antisymmetric. These will be labeled ϕ_1 and ϕ_2 , with respective energies ε_{b1} and ε_{b2} , and $\varepsilon_{b1} \leq \varepsilon_{b2}$. It is assumed throughout that the bound electron initially occupies ϕ_1 . The energy of the sys-

tem therefore lies in the band for an electron propagating in ideal leads and another electron bound in ϕ_1 , that is, $E = \varepsilon_{b1} + 2t \cos k_1$. If this band of energies overlaps with the band for an electron propagating in ideal leads and an electron bound in the excited state ϕ_2 , there is the possibility of inelastic scattering. Starting at the threshold energy $\varepsilon_{b2} - 2t$, the scattering process can end with the bound electron excited to the energy ε_{b2} and the propagating electron departing with the altered wave vector k_2 , as dictated by the “ ϕ_2 plus propagating electron” band. Below the threshold energy scattering is therefore entirely elastic. This will be referred to as the elastic regime. Above the threshold energy, the propagating electron will in general scatter into a combination of states with wave vector k_1 and states with wave vector k_2 (and the bound electron will occupy a corresponding combination of ϕ_1 and ϕ_2). This will be referred to as the inelastic regime. The probability of transmission into a given channel, the partial transmittivity, is given by

$$P(E) = \frac{\sin k_i}{\sin K} |p_{k_i}|^2, \quad (20)$$

where k_i is the wave vector for the propagating electron in channel i , K is the wave vector for the propagating electron in the channel in which it was initialized (in this study always k_1), and p_{k_i} is the amplitude of the propagating electron in channel i . In this study, $i=1, 2$.

The correct form for the concurrence between the propagating and the bound electron when they are in the inelastic-elastic superposition state found in the inelastic regime is given by the formula⁴⁰ of Ramšak *et al.*,

$$C = \frac{\left| \int [p_{sing}^2(k) - p_{trip}^2(k)] |\phi_k|^2 dk \right|}{\int [|p_{sing}(k)|^2 + |p_{trip}(k)|^2] |\phi_k|^2 dk}. \quad (21)$$

Again, this applies for the starting spin state $|\uparrow\downarrow\rangle$. For inelastic scattering in the two binding site system, we have $|\phi_k|^2 = \delta(k_1) + \delta(k_2)$. The concurrence is hence

$$C = \frac{|p_{k_1,sing}^2(k_1) + p_{k_2,sing}^2(k_2) - p_{k_1,trip}^2(k_1) - p_{k_2,trip}^2(k_2)|}{|p_{k_1,sing}(k_1)|^2 + |p_{k_2,sing}(k_2)|^2 + |p_{k_1,trip}(k_1)|^2 + |p_{k_2,trip}(k_2)|^2}. \quad (22)$$

The approach of Ramšak *et al.* also facilitates the calculation of concurrence in the system of degenerate leads. Considering only transmitted electrons, there are now three domains for concurrence. In the first two, only electrons transmitted by one or the other of the sets of leads are considered for purposes of entanglement with the bound electron. In the third domain, any electron transmitted via either set of leads is considered. The concurrence for each of these domains is calculated by incorporating the appropriate singlet and triplet scattering amplitudes into the concurrence formula Eq. (7). For example, concurrence between the bound electron and an electron transmitted via either lead set is given (in the elastic regime) by

$$C = \frac{|p_{1,sing}^2 + p_{2,sing}^2 - p_{1,trip}^2 - p_{2,trip}^2|}{|p_{1,sing}|^2 + |p_{2,sing}|^2 + |p_{1,trip}|^2 + |p_{2,trip}|^2}. \quad (23)$$

As previously noted, scattering behavior is calculated separately for the singlet and triplet components of the two-electron wave function in this study by, respectively, symmetrizing and antisymmetrizing the spatial wave function. If ε_0 is sufficiently high, the scattering behavior will approximate to the behavior in the limit $\varepsilon_0 \rightarrow -\infty$. A qualitative understanding of the scattering behavior of one electron from a second electron, bound at a doubly degenerate binding site, with or without degenerate leads, can be arrived at by analyzing the singlet and triplet scattering in the limit $\varepsilon_0 \rightarrow -\infty$. In this limit, ϕ_1 and ϕ_2 become $\frac{1}{\sqrt{2}}(1, 1)$ and $\frac{1}{\sqrt{2}}(1, -1)$ in the basis of the two binding sites. Apart from separable scattering states which are incorporated into the boundary conditions, the only two-electron states that need be accounted for in this limit are those in which both electrons reside on one or the other of the binding sites. Labeling sites 1 and 2, the relevant single electron states are $|1\rangle$ and $|2\rangle$. In the triplet (spatially antisymmetric) state, scattering is therefore via just one spatial state: $|1\ 2\rangle$, with energy $2\varepsilon_0 + V$. In the singlet (spatially symmetric) state, scattering is via three spatial states: $|1\ 1\rangle$, $|1\ 2\rangle$, and $|2\ 2\rangle$ with energies $2\varepsilon_0 + U$, $2\varepsilon_0 + V$, and $2\varepsilon_0 + U$, respectively.

Singlet scattering in the limit $\varepsilon_0 \rightarrow -\infty$ can be analyzed by diagonalizing the space of these three states, viewing the propagating electron as scattering through three decoupled states. The energies of the new, decoupled two-electron states are

$$\varepsilon'_{1,3} = 2\varepsilon_0 + \frac{U+V}{2} \pm \frac{\sqrt{(U-V)^2 + 8t_c^2}}{2}, \quad \varepsilon'_2 = 2\varepsilon_0 + U. \quad (24)$$

In the elastic regime and the limit $\varepsilon_0 \rightarrow -\infty$, transmission can therefore be characterized by amplitudes of the form of Eq. (8), with appropriately modified coupling between the central states and the lead. One term of the form of Eq. (8) will describe the triplet (antisymmetric) transmission, and three such terms will describe the singlet (symmetric) transmission. In the latter transmission spectrum, the overall amplitude will have the form $p = p_1 - p_2 + p_3$, where p_{1-3} are expressions of the form of Eq. (8) corresponding to each of the three decoupled two-electron states. Depending on the value of V (and recalling that for the purposes of this study it is assumed that $\varepsilon_{b1} - 2t < 2\varepsilon_0 + U < \varepsilon_{b1} + 2t$), either one or no peaks will appear in the triplet transmission spectrum, and either two or three peaks will appear in the singlet transmission spectrum, corresponding to those of the two-electron states with energies that will result in quasibound states. The singlet transmission spectra of the doubly degenerate binding site and the second lead set of the degenerate leads system will display an antiresonance, as in the single-electron case. This is the result of transmission via the second decoupled two-electron state cancelling transmission via the other two states, $p_2 = p_1 + p_3$.

In this study, the calculated scattering behavior and the resultant entanglement between the scattered electron and the

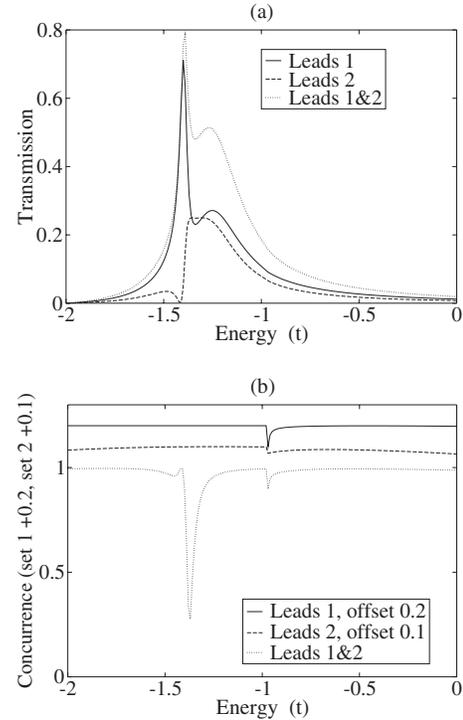


FIG. 5. (a) Singlet scattering, first and second lead sets, and overall for the degenerate leads system. $\varepsilon_0 = 10t$, $t' = t/4$, $t'' = t/8$, $t_c = t/2$, $U = -(\frac{7}{4}t + \varepsilon_0)$, and $V = 0$. (b) Concurrence for electrons transmitted through the first lead set (offset by 0.2), through the second lead set (offset by 0.1) and for electrons transmitted through either lead set. The boundary of the inelastic regime is at $E - \varepsilon_{b1} \approx -1$.

bound electron are presented for two differing parameter sets. In the first $\varepsilon_0 = 10t$, $t' = t/4$, $t'' = t/8$, $t_c = t/2$, $U = -(\frac{7}{4}t + \varepsilon_0)$, and $V = 0$. With these parameters, all resonances in transmission lie within the elastic regime. The binding-site potential ε_0 is large enough that qualitative comparisons with the limit $\varepsilon_0 \rightarrow \infty$ are valid. Since $V = 0$, only two resonant peaks are expected in the singlet transmission spectrum and none at all in the triplet transmission spectrum. The singlet transmission spectrum will be qualitatively similar to the single-electron transmission spectrum for a value of ε_0 similar to the value of $\varepsilon_0 + U$ used here.

Figure 5 shows the singlet transmission probabilities, and concurrences, for one electron scattering from another bound within the degenerate-leads system. Using these parameter values, triplet transmission probabilities were uniformly very low due to the lack of resonant transmission. Results for the doubly degenerate binding-site system will be qualitatively similar to those for the second lead set shown here, although transmission probabilities will be four times higher. The boundary of the inelastic regime is $E - \varepsilon_{b1} \approx -1$.

As with the single electron case, two peaks are found in the transmission spectra of both lead set 1 and lead set 2. Transmission through lead set 2 also contains an antiresonance, as anticipated from the single electron case. Within the elastic regime, concurrence is overall high, although it is lower (and suffers a sharp drop) when measured between electrons transmitted through both channels, and the bound electron. Even in this case, a peak to $C \approx 1$ is found, corre-

sponding to a peak in transmission through lead set 1. High concurrence is therefore possible along with a high probability of transmission. Concurrence drops off in the inelastic regime (as singlet transmission drops dramatically toward the same order of magnitude as triplet transmission), but since transmission probability is generally very low in this regime, this is not important.

Scattering behavior is less straightforward in the inelastic regime. Once again taking the limit $\varepsilon_0 \rightarrow -\infty$, each of the binding-site two-electron states is now effectively coupled to two sets of boundary condition states. In one set, the propagating electron is scattered elastically. In the other, it is scattered inelastically, leaving the bound electron in ϕ_2 and the propagating electron moving according to the wave vector k_2 . The scattering amplitude for elastic scattering from a single, decoupled state is

$$p_{\tau,k_1} = \frac{i \sin k_1}{\frac{t(\varepsilon'_\tau - E)}{2\alpha\beta} + \frac{\alpha}{\beta} e^{ik_1} + \frac{\beta}{\alpha} e^{ik_2}}, \quad (25)$$

where α is the coupling of the binding-site state to the elastic scattering boundary states, β is the coupling to the inelastic scattering boundary states, and ε'_τ is the energy of the binding site state. All of these parameters are known functions of ε_0 , t , t' , t'' , t_c , U , and V . The main difference between this amplitude and the general scattering amplitude [Eq. (8)] for the elastic regime is the introduction of the term $\frac{\beta}{\alpha} e^{ik_2}$ into the denominator, representing dependence on the inelastically scattered wave vector k_2 .

In general, this term suppresses the amplitude p_{τ,k_1} . The expression for the position of the antiresonance, $p_2 = p_1 + p_3$, no longer has a solution for any real energy. The antiresonance in the transmission spectrum of the doubly degenerate binding site and the second lead set of the degenerate leads system therefore vanishes in the inelastic scattering regime. The peaks associated with each term of the form of Eq. (25) are not resonant, and in the case of states with weak coupling, such peaks can no longer be distinguished. Finally, if $\alpha \rightarrow 0$, the term in question is completely suppressed. It can be shown that this occurs in the limit $\varepsilon_0 \rightarrow -\infty$ when $t_c = V - U$.

The scattering amplitude for inelastic scattering through a single, decoupled state is similar in form to Eq. (25). Both the elastic and the inelastic channels hence have similar transmission spectra, with a single nonresonant peak given by each term of the form of Eq. (25), which may be suppressed by sufficiently weak coupling to the binding-site states. The triplet transmission spectrum will therefore have either one or no peaks, and the singlet transmission spectrum will have between one and three peaks (but no antiresonance) depending on the relative strengths of the couplings.

The second and contrasting parameter set for which data are presented is $\varepsilon_0 = 10t$, $t' = t/4$, $t'' = t/8$, $t_c = t/2$, and $U = V = \varepsilon_0$. Once again, the binding-site potential ε_0 is large enough that qualitative comparisons with the limit $\varepsilon_0 \rightarrow -\infty$ are valid, and the boundary of the inelastic regime is again $E - \varepsilon_{b1} \approx -1$. Given these parameter values, a peak in the triplet transmission spectrum and up to three peaks in the singlet

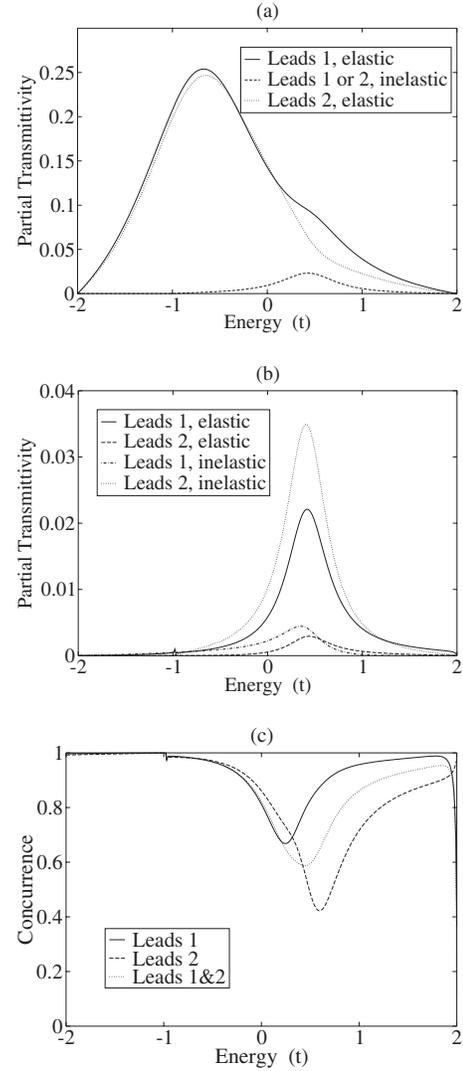


FIG. 6. (a) Singlet scattering and first and second lead sets for the degenerate leads system. $\varepsilon_0 = 10t$, $t' = t/4$, $t'' = t/8$, $t_c = t/2$, and $U = V = -\varepsilon_0$. (b) Triplet scattering for the same system. (c) Concurrence after scattering for the starting state $|\uparrow\downarrow\rangle$. The boundary of the inelastic regime is at $E - \varepsilon_{b1} \approx -1$.

transmission spectrum (both in elastic and inelastic transmissions) might be expected, all of which will lie in the inelastic regime. Transmission spectra and concurrence data are presented for this parameter set in Fig. 6.

A single peak is indeed found in the triplet transmission spectra at approximately the same energy in both lead sets and in the elastic and inelastic channels. The peak is also close to the energy of the two-electron binding-site state through which the electron is supposed to resonantly scatter, $2\varepsilon_0 + V$. In the singlet transmission spectra, however, there is a single peak that appears in the elastic transmission spectra, and a single peak at a different energy that appears in the inelastic transmission spectra. The reasons for the nonappearance of a further two peaks in both channels are the couplings of the three decoupled binding-site two-electron states to the leads. Given that $U = V$, the energies of the decoupled states and their couplings to the leads in either chan-

nel are approximately (exactly in the limit $\varepsilon_0 \rightarrow -\infty$) given by

$$\text{State 1: } \varepsilon'_1 = 2\varepsilon_0 + U - \sqrt{2}t_c,$$

$$\alpha = \left(\frac{1}{\sqrt{2}} - 1 \right) (t' + t''),$$

$$\beta = \left(\frac{1}{\sqrt{2}} + 1 \right) (t'' - t').$$

$$\text{State 2: } \varepsilon'_2 = 2\varepsilon_0 + U,$$

$$\alpha = (t' - t''),$$

$$\beta = (t' + t'').$$

$$\text{State 3: } \varepsilon'_3 = 2\varepsilon_0 + U + \sqrt{2}t_c,$$

$$\alpha = \left(\frac{1}{\sqrt{2}} + 1 \right) (t' + t''),$$

$$\beta = \left(\frac{1}{\sqrt{2}} - 1 \right) (t'' - t'). \quad (26)$$

Again, α is the coupling of the binding-site state to the elastic scattering boundary states, β is the coupling to the inelastic scattering boundary states, and ε'_τ is the energy of the decoupled binding site state. As noted [Eq. (25)], scattering via one of these states into a given channel is suppressed both by weak site-lead coupling to that channel and by strong site-lead coupling to the other channel. Coupling to the inelastic channel from state 3 is weak, while coupling to the elastic channel is strong, so scattering via state 3 is the major contributor to elastic channel transmission (yielding the peak seen in the elastic channel spectra), but is not distinguishable in the inelastic channel. The converse is true of scattering via state 2, and it is this that gives rise to the single peak seen in the inelastic transmission spectra. Scattering via state 1 is suppressed in both channels. Modification of V from strict equality with U reveals that this a consequence of the disappearance of coupling to the elastic channel, $\alpha \rightarrow 0$, discussed previously. The parameters used here, $U=V$ and $t_c=t/2 \neq 0$, do not meet the criterion $t_c=V-U$ established for the limit $\varepsilon_0 \rightarrow -\infty$. This is a case in which the results for finite ε_0 diverge somewhat from those in the limit $\varepsilon_0 \rightarrow -\infty$.

The main feature of the concurrence, measured at either lead set or at both lead sets, is a drop in the same energy region as the peaks in the triplet transmission spectra. This is a consequence of the singlet and triplet transmission probabilities becoming closer, leading to increasing mixing between the two in the transmission regime. The concurrence also suffers a notable (if slight) drop at the boundary between the elastic and inelastic regimes. As a result, although concurrence is still high (~ 0.95) in the region of the transmission peak in the singlet transmission spectra, there is no part of the energy band in which concurrence at ≈ 1 is combined with high transmission probability. This makes scattering

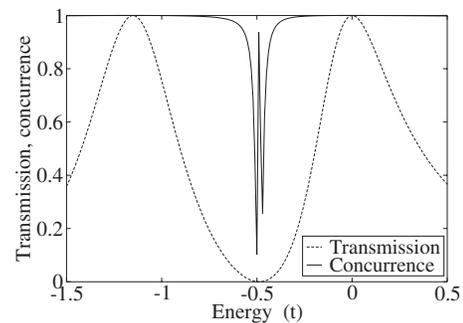


FIG. 7. Singlet transmission probability and concurrence for a doubly degenerate impurity. $\varepsilon_0 = -10t$, $t' = t'' = t/4$, $t_c = 0.15t$, $U = -\varepsilon_0$, and $V = -(t + \varepsilon_0)$.

from an electron at a degenerate binding site in the inelastic regime disadvantageous for creating entanglement, as compared to scattering in the elastic regime, and especially as compared to the nondegenerate case. However, the high probability of transmission (in the case of the degenerate impurity with nondegenerate leads, this will approach 1) combined with high, although not unity, concurrence means that (at least with this parameter set) the system is still effective in generating entanglement.

A further parameter regime which is of interest to the entanglement of a propagating electron with an electron bound at a degenerate binding site is $|\varepsilon_0| \gg t$, $t' = t'' \ll t$, $\varepsilon_{b1} - 2t < 2\varepsilon_0 + U$, and $2\varepsilon_0 + V < \varepsilon_{b1} + 2t$. As noted for the single-electron case, equalizing the site-lead couplings, $t' = t''$, decouples the antisymmetric combination of the binding sites, leaving (in the single electron case) a single resonant peak in the transmission spectrum. In the case of two electron scattering, this equality has three consequences. The first is that the antisymmetric excited state of the bound electron is completely decoupled from the leads in the singlet (spatially symmetric) configuration, so there is no inelastic regime. The second is that the single two-electron binding site state available to the triplet (spatially antisymmetric) configuration is also decoupled from the leads, so that (recalling that $|\varepsilon_0| \gg t$) there will be no resonant scattering in the triplet configuration. The final consequence is that one of the three decoupled two-electron binding-site states available to the singlet spin state is also decoupled from the leads. As a result, there are a maximum of two resonances that can occur in the singlet transmission, and none of that can occur in triplet transmission. In the parameter regime $\varepsilon_{b1} - 2t < 2\varepsilon_0 + U$ and $2\varepsilon_0 + V < \varepsilon_{b1} + 2t$, both possible resonances will occur in singlet transmission.

The consequences of scattering in this regime for transmission behavior and concurrence are illustrated by the singlet scattering spectrum and the concurrence (again, from the starting state $|\uparrow\downarrow\rangle$) for the parameter set $\varepsilon_0 = -10t$, $t' = t'' = t/4$, $t_c = 0.15t$, $U = -\varepsilon_0$, and $V = -(t + \varepsilon_0)$. These data are plotted in Fig. 7, in this case for the doubly degenerate binding site without lead degeneracy. Triplet transmission is very low across the entire band.

There are two resonances in singlet transmission and an antiresonance (at which transmission via the two binding-site states coupled to the leads cancels out). Concurrence is high

across the band, with the exception of the region of the antiresonance. Most importantly, concurrence approaches one in the region of both the resonances. This means that there are two energies at which high propagating-bound concurrence is combined with a very high probability of singlet transmission, rather than (as in the nondegenerate case) one energy. The generation of entanglement between a static and a flying qubit is therefore easier in this system than in its nondegenerate analog.

V. CONCLUSIONS

In conclusion, a generalized real-space Anderson model has been used to model two-electron scattering behavior in one-dimensional systems incorporating degeneracy of both binding centres and ideal leads, and the static-flying qubit entanglement that results from such scattering. Inelastic scattering in such systems has been addressed. Systems with degenerate leads act as models for the degenerate first conduction channel of carbon nanotubes, while a degenerate binding site is a model for an orbitally degenerate carbon nanotube quantum dot.

In the elastic regime and with little Coulombic interaction between components of the degenerate binding sites, it has been shown that the qualitative features of the single-electron scattering are preserved. One or two resonant peaks are observed, along with an antiresonance, in the singlet transmission spectrum. Triplet transmission is uniformly low, so the resonant and antiresonant features of the transmission spectrum are spin dependent. This is particularly interesting in the context of systems with degenerate leads, since only one set of leads is found to display antiresonant behavior in the singlet state, raising the possibility of spin filtering by selective transmission. In addition, the reappearance of the antiresonant structure in the two-electron transmission spectrum provides a few-electron basis for the antiresonant effects recently observed in quasi-one-dimensional structures.^{33,42–44} Concurrence in this regime is not uniformly high, but approaches one in regions of high transmission, indicating that such systems may be useful for the generation of entanglement.

Raising the Coulombic interaction between components of the degenerate binding site raises triplet transmission and

therefore lowers concurrence in parts of the energy band. In the inelastic scattering regime, components of the singlet transmission behavior are suppressed. This suppression differentiates between the elastic and inelastic channels. The result is large drops in concurrence in some parts of the band, while overall concurrence is lower in the inelastic than in the elastic regime. In addition, transmission as a whole is lower due to the coupling of binding site states to multiple scattering channels.

Beyond this, systems with degenerate leads are overall less useful than those with nondegenerate leads since the branching of the paths available to the scattered electron lowers overall transmission.

In general, degeneracy of the binding sites or the leads therefore makes the generation of entanglement between the spins of a propagating electron and a bound electron harder to generate than in the nondegenerate case. For most parameter values, it is found that either overall transmission probability or concurrence are lowered relative to the nondegenerate case. Acceptable values of transmission probability and concurrence may nevertheless be found at appropriate energies of propagation. The lowering of transmission and concurrence is particularly noticeable in the inelastic scattering regime. The most clear exception to this is the parameter regime in which $t' = t''$. In this regime, no inelastic scattering occurs and if the Coulombic interaction between components of the degenerate binding site is sufficient (that is, if $\epsilon_{b1} - 2t < 2\epsilon_0 + V < \epsilon_{b1} + 2t$), then two resonances in singlet transmission with accompanying peaks in concurrence (to $C \approx 1$) will be produced, providing two energies at which a high degree of entanglement can be produced with maximum probability, and hence making the generation of entanglement easier than in the non-degenerate case.

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