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Interacting resonant level coupled to a Luttinger liquid: Universality of thermodynamic properties

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Abstract – We investigate a model of a single resonant level coupled to the edge of a quantum wire in the Luttinger-liquid phase or to the middle of a chiral Luttinger liquid via both tunneling and a contact interaction. Utilizing the Yuval-Anderson approach, we map this model onto a classical 1D Coulomb gas in which all the details of both the interactions in the lead and the level-lead interaction enter only through the corresponding Fermi-edge singularity exponent, which we explicitly evaluate using the Bethe ansatz solution for a particular model of the lead. Thus the population, dynamical capacitance and level entropy are universal in the sense of being equal for models with interactions differing in magnitude and even in sign. We demonstrate this to hold quantitatively using density matrix renormalization group calculations. Since the Coulomb gas description is of the single-channel Kondo type, we infer that the universality we found implies that Luttinger-liquid physics has no qualitative effect on these properties, in contrast with perturbative results.

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Introduction. – Understanding the properties of strongly correlated systems has been one of the main fields of investigation in condensed matter physics in recent years. An important class of such problems is that of quantum impurities, *i.e.*, systems with a finite number of degrees of freedom coupled to reservoirs of non-interacting particles, the best known examples of which are the Kondo and Anderson models [1] and the spin-boson model [2]. Another important type, for which non Fermi-liquid physics is well established, is that of one dimensional electronic systems. When no symmetry is spontaneously broken, the low energy physics of those systems is described by the Luttinger-liquid (LL) theory, where the quasiparticles are bosonic modes of density (or, in a dual description, phase) fluctuations [3]. It is then natural to try to bring these two themes together, by studying quantum impurities coupled to LLs: from the quantum impurity perspective, the reservoir now has a non-trivial physics of its own; from the LL point of view, this gives a way to probe the intricate physics of the electrons which are coupled to the impurity (and not the relatively simple behavior of the weakly inter-

acting bosons). Besides these fundamental motivations, quantum impurities (*e.g.*, quantum dots) and LLs (*e.g.*, quantum wires), are the basic ingredients of nano-scale circuits, so that understanding them has a profound importance for applications. Although such models have been studied theoretically for some time, most effort has been concentrated at understanding transport properties [3,4]; other phenomena have usually received only scant attention [5–11].

Model. – The simplest possible system to study these effects is that of a single level coupled to the edge of a LL (which can be realized by, *e.g.*, lithographically defining a small quantum dot at the end of a quantum wire, or by coupling a metallic grain to the edge of a metallic nanowire, or an impurity atom to the end of a carbon nanotube), or, equivalently, to the middle of a chiral LL (*e.g.*, a dot near the edge of a fractional quantum hall bar) [12]. We include contact interaction between the level and the lead. Here transport properties are not relevant; however, many other interesting questions can be investigated. In this letter we concentrate on thermodynamic properties: the level population, its dynamical capacitance (which can be probed experimentally by capacitively

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coupling the system to a quantum point contact) and the level contribution to the entropy and specific heat. We demonstrate, both analytically and numerically, that these properties show universality, and depend on the different interactions only through a single parameter, the Fermi edge singularity exponent of the system. Using an analogy to the single-channel Kondo problem, we show this universality to imply that these physical quantities have an essentially Fermi liquid like behavior, which is affected only quantitatively, but not qualitatively, by LL physics.

The system is described by the following Hamiltonian:

$$H = H_{\text{lead}}\{\psi^\dagger(x), \psi(x)\} + \varepsilon_0 d^\dagger d - [\gamma_{\text{ll}} d^\dagger \psi(0) + \text{H.c.}] + \frac{\lambda_{\text{ll}}}{2} \left(d^\dagger d - \frac{1}{2} \right) [\psi^\dagger(0)\psi(0) - \psi(0)\psi^\dagger(0)], \quad (1)$$

where d , $\psi(x)$ are Fermi operators of the level and the lead, respectively, ε_0 is the bare level energy, γ_{ll} is the level-lead tunneling matrix element, and λ_{ll} is the strength of the level-lead interaction. At low energies the lead Hamiltonian assumes the Tomonaga-Luttinger form. It can then be written in terms of two Bose fields $\Theta(x)$ and $\Phi(x)$ obeying the commutation relation $[\Theta(x), \Phi(x')] = i\pi\theta(x-x')$ [$\theta(x)$ is the step function], and the boundary condition $\Theta(0) = 0$ [3]:

$$H_{\text{lead}} = \frac{v}{2\pi} \int_0^\infty \left\{ \frac{1}{g} [\partial_x \Theta(x)]^2 + g [\partial_x \Phi(x)]^2 \right\} dx, \quad (2)$$

where g and v are the usual LL interaction parameter and excitation velocity, respectively. The electron density equals $\partial_x \Phi/\pi$, and the electron annihilation operator at the the edge of the lead can be expressed in the bosonic language as $\psi(0) = \chi e^{i\Phi(0)}/\sqrt{2\pi a}$, using a Majorana Fermi operators χ and a short distance cutoff (*e.g.*, a lattice spacing) a .

Yuval-Anderson approach and universality. –

Using the Yuval-Anderson approach [13], in either the canonical [14] or the path-integral [15] formulations, we expand the partition function to all orders in γ_{ll} and evaluate the resulting terms. The expression thus obtained is a sum over all possible imaginary time histories of the level, which fluctuates between the empty and filled states. We then obtain the expression

$$Z = \sum_{\substack{N=0 \\ \sigma=\pm 1}}^\infty \left(\frac{\Gamma_0 \xi_0}{\pi} \right)^N \int_0^{\tau_2 - \xi_0} \frac{d\tau_1}{\xi_0} \int_0^{\tau_3 - \xi_0} \frac{d\tau_2}{\xi_0} \dots \int_0^{\tau_{2N} - \xi_0} \frac{d\tau_{2N-1}}{\xi_0} \int_0^\beta \frac{d\tau_{2N}}{\xi_0} \exp[-\mathcal{S}(\{\tau_i\}, \sigma)], \quad (3)$$

where ξ_0 is a short time (ultraviolet) cutoff, Γ_0 is the (renormalized) level width (an expression for which is given below), and β is the inverse temperature of the original problem. This expression thus has the form of a classical grand canonical partition function of a one dimensional gas of particles (“Coulomb gas”) residing

on a circle of circumference β , with fugacity $\sqrt{\Gamma_0 \xi_0/\pi}$. Each particle is assigned a positive (negative) charge if it corresponds to hopping of an electron from the lead to the level (vice versa). The charges must thus be alternating, with an overall charge neutrality. Hence, a configuration is completely specified by the sign of the first charge (denoted by σ in the above expression) and by the positions of the particles. The action of this classical system consists of two terms:

$$\mathcal{S}(\{\tau_i\}, \sigma) = \alpha_{\text{FES}} \sum_{1 \leq i < j \leq 2N} (-1)^{i+j} \ln \left\{ \frac{\pi \xi_0 / \beta}{\sin[\pi(\tau_j - \tau_i)/\beta]} \right\} + \varepsilon_0 \left[\beta \frac{1-\sigma}{2} + \sigma \sum_{1 \leq i \leq 2N} (-1)^i \tau_i \right]. \quad (4)$$

The first term is an interaction between the particles, with the form of a Coulomb interaction between charged rods, and a coefficient (charge squared) α_{FES} , the Fermi edge singularity exponent of our problem (by which we refer to twice the scaling dimension of $d^\dagger \psi(0)$ for $\lambda_{\text{ll}} = 0$). We discuss its value below. If the lead has a finite length L but the temperature is zero, one should substitute $L/(iv)$ for β inside the logarithm, whereas at finite temperature the sine is replaced by an elliptic function [16]. The second term in the action of the classical system corresponds to the energetic cost of filling the level, and resembles the effect of an electric field applied on the charges.

We thus see that the partition function depends on the original model only through three parameters: Γ_0 , ε_0 and α_{FES} . As we show below, the latter, in particular, contains the main effects of the interactions, both in the lead and between the level and the lead. This implies a *universality* in this system. We use this term here to refer to the fact that many of the properties of the system depend only on these three parameters, so that they will be the same for very different systems, with different strengths and signs of interactions, provided these three parameters are indeed the same. The properties which exhibit universality are the thermodynamic ones, *e.g.*: the level population and its correlation functions (or, equivalently, the static and dynamic level capacitance), and the level contributions to the entropy and the specific heat.

Since the universality is based on the Yuval-Anderson description, it is important to understand the limitations of the latter. The derivation of the Coulomb gas representation assumes that the correlation functions of the tunneling term $d^\dagger \psi(0)$ behave as power laws in time. While this is correct for the Tomonaga-Luttinger Hamiltonian (2), any particular model of a one-dimensional lead will differ from it by terms which are irrelevant at low-energies (or, equivalently, long times) in the renormalization group sense. This will affect the correlation functions in two ways: i) At long times they will retain the power law form, but with renormalized power and prefactor. ii) At short times the power law form itself could be modified. The

first effect does not change the form of the Coulomb gas expansion (or the resulting universality), and can be accounted for by using the appropriate renormalized values of the Coulomb gas parameters α_{FES} and Γ_0 . These values are discussed in the following section. The second effect, on the other hand, could have resulted in a real limitation of the Anderson-Yuval description. However, numerical data presented below shows that, to a very high degree of accuracy, this has no quantitative effect, except in the vicinity of the transition points from the LL phase to non-metallic phases (where perturbations to the Tomonaga-Luttinger Hamiltonian become relevant).

Coulomb gas parameters. — Following these comments, we now discuss in more details the parameters appearing in the Coulomb gas form of the partition function. In the case where the lead is noninteracting, we have the usual resonant level model, for which it is known that $\alpha_{\text{FES}} = (1 - \frac{2}{\pi}\delta)^2$ and $\Gamma_0 = \pi|\gamma_{\text{ll}}|^2\nu_0 \cos(\delta)$, where $\delta = \tan^{-1}(\pi\nu_0\lambda_{\text{ll}}/2)$ is the phase shift of the electrons in the lead caused by their interaction with the level, and ν_0 is the local density of states at the end of the lead [17,18]. When there are nonvanishing interactions both in the lead and between the level and the lead, the situation is more complicated. From bosonization [3] we obtain (since there is no backscattering in this problem) $\alpha_{\text{FES}} = (1 - g\lambda_{\text{ll}}/\pi v)^2/g$, and $\Gamma_0 = \pi|\gamma_{\text{ll}}|^2\nu_0$. If we go to the limit of a noninteracting lead (with $\nu_0 = 1/(\pi v)$ taking into account both the left-and right-going branches), we see that in the bosonization treatment expressions that should contain the phase shift δ are replaced by their leading-order dependence on λ_{ll} . This is the result of irrelevant corrections to the LL Hamiltonian (2), in this case — the band curvature.

On the other hand, from boundary conformal field theory arguments [19] it follows that $\pi v\alpha_{\text{FES}}/L$ is equal to the $1/L$ correction to the difference between the two energies: the energy of a lead with no attached level but with potentials of strengths $\pm\lambda_{\text{ll}}/2$ applied on its two edges, and the energy of that lead with one electron extracted and a potential of strength $\lambda_{\text{ll}}/2$ applied on both ends. It may thus be calculated numerically, or even analytically when an exact solution is available. Let us consider, for example, a discrete realization of the lead as a half-filled tight-binding chain with nearest-neighbor interactions:

$$H_{\text{TBI}} = \sum_{i=1}^{\infty} \left[-tc_i^\dagger c_{i+1} + \text{H.c.} + U(n_i - \frac{1}{2})(n_{i+1} - \frac{1}{2}) \right], \quad (5)$$

where c_i is the Fermi operator at the lead's i -th site, $n_i = c_i^\dagger c_i$ is the corresponding number operator, while t and U are the nearest-neighbor hopping and interaction strengths along the chain. The LL parameters of this model are $g = \pi/[2\cos^{-1}(-\Delta)]$, and $v/(ta) = \pi\sqrt{1-\Delta^2}/\cos^{-1}\Delta$, with $\Delta \equiv U/2t$ and a denoting the lattice spacing [3]. The full Hamiltonian

Table 1: Parameters appearing in the Coulomb gas model, eqs. (3) and (4). See the text for further details.

	Non-interacting lead	Bosonization	General model
α_{FES}	$(1 - \frac{2}{\pi}\delta)^2$	$\frac{1}{g}(1 - \frac{g\lambda_{\text{ll}}}{\pi v})^2$	$\frac{1}{g}(1 - g\frac{2}{\pi}\delta_{\text{eff}})^2$
Γ_0	$\pi \gamma_{\text{ll}} ^2\nu_0 \cos(\delta)$	$\pi \gamma_{\text{ll}} ^2\nu_0$	$\pi \gamma_{\text{ll}} ^2\nu_0 \cos(\delta_{\text{eff}})$

(including the level) is now

$$H_{\text{TB}} = H_{\text{TBI}} + \varepsilon_0 d^\dagger d - (t_{\text{ll}} c_1^\dagger d + \text{H.c.}) + U_{\text{ll}}(d^\dagger d - \frac{1}{2})(c_1^\dagger c_1 - \frac{1}{2}), \quad (6)$$

where the level-lead couplings are related to their continuum counterparts by $\gamma_{\text{ll}} = t_{\text{ll}}\sqrt{a}$, and $\lambda_{\text{ll}} = U_{\text{ll}}a$. This model of the lead (or its equivalent, the XXZ spin chain [3]) is exactly solvable by the Bethe ansatz even for a finite size system and in the presence of potentials at the boundary [20,21]. Hence, an analytic expression for α_{FES} can be found in this case

$$\alpha_{\text{FES}} = \frac{1}{g} \left[1 - \frac{2g}{\pi} \tan^{-1} \left(\frac{U_{\text{ll}}}{\sqrt{(2t)^2 - U^2}} \right) \right]^2. \quad (7)$$

It then seems natural to identify $\delta_{\text{eff}} = \tan^{-1} \left(\frac{U_{\text{ll}}}{\sqrt{(2t)^2 - U^2}} \right)$ as an effective phase shift, which reduces to the usual phase shift when the lead is noninteracting. We may thus expect that for a general model we can write $\alpha_{\text{FES}} = \frac{1}{g} (1 - \frac{2g}{\pi}\delta_{\text{eff}})^2$, for some effective phase shift $\delta_{\text{eff}} \in [-\pi/2, \pi/2]$, so that Γ_0 will be given by $\pi|\gamma_{\text{ll}}|^2\nu_0 \cos(\delta_{\text{eff}})$. In the following we will confirm these results quantitatively by our numerical data. The discussion in the last two paragraphs is summarized in table 1.

We note in passing that the mapping into the Coulomb gas can be easily extended to include the case of an Ohmic environment coupled to the level. The only effect of this on the analysis is modifying the parameter α_{FES} by adding to it the impedance of the environment divided by the quantum resistance h/e^2 [6]. Hence, all our results apply to this case too. The universality is thus seen to have an even broader scope of applicability.

Numerical results. — Let us now turn to a numerical test of the universality. As we explained above, this enables us to show that although the mapping to a Coulomb-gas applies rigorously only to the low-frequency (long-time) behavior, we have found that universality holds *quantitatively*, at least when irrelevant perturbations of the LL are not too strong. To this end we have performed density matrix renormalization group (DMRG) [22] calculations on the half-filled tight-binding realizations of the system, eqs. (5) and (6). Up to 256 block states were kept in each iteration. In fig. 1 we show the differential capacitance

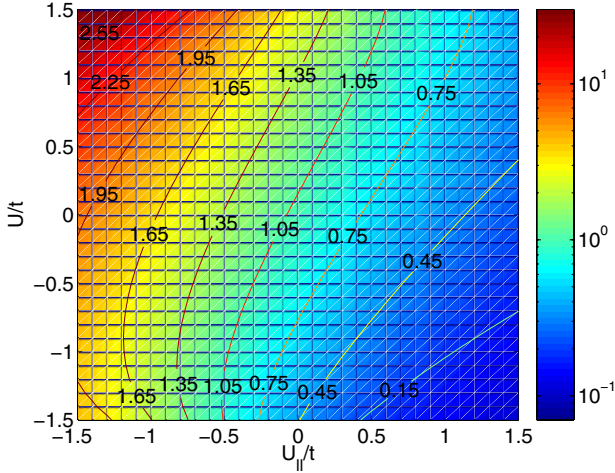


Fig. 1: (Color online) A color map of the differential capacitance (divided by the noninteracting value) obtained by DMRG at half filling, as a function of the interactions in the lead and between the level and the lead, with contours of constant α_{FES} superimposed. It can be seen that the effect of all the interactions comes only through this parameter, confirming universality. See the text for further details.

$\partial n / \partial \varepsilon_0$ at $\varepsilon_0 = 0$ in a color map as a function of both the level-lead interaction and the interaction in the lead. In all cases we have kept $\Gamma_0 = 10^{-4}t$ and $L = 50v/t$, modifying t_{\parallel} and L accordingly, so as to keep all the parameters of the Coulomb gas constant except α_{FES} . On the color map we superimposed a contour plot of α_{FES} , taken from eq. (7). It is indeed seen that the contours of constant α_{FES} are also contours of constant differential capacitance, confirming the important role of the former in determining the behavior of the system. Deviations are seen only for quite strong interactions, where irrelevant terms in the Hamiltonian are initially quite strong (and are not renormalized to zero because of the finite system size), and thus modify the results quantitatively. To appreciate this one should remember that for $|U| > 2t$ the system is no longer a LL [but becomes charge density wave (phase separated) for positive (negative) U]; whereas for $|U_{\parallel}| > 2t$ the potential of $\pm U_{\parallel}/2$ felt at the last site of the lead when the level is full (empty) is strong enough to form a bound state. Both of these effects are not included in our treatment.

A more detailed comparison is made in fig. 2. Here we show the full dependence of the level population on its energy. The population curves corresponding to different α_{FES} values are presented, and on each such curve there are symbols of four types, denoting the numerical results on four different models: a) a non-interacting lead with nonzero level-lead interaction; b) a lead with nearest-neighbor interactions but zero level-lead term; c) a system with both nonzero U_{\parallel} and nearest-neighbor interaction in the lead (which serves as a test to eq. (7) and the subsequent discussion); d) a lead with next-nearest-neighbor interactions of strength V in addition to the nearest-neighbor interactions (but vanishing U_{\parallel}), *i.e.*,

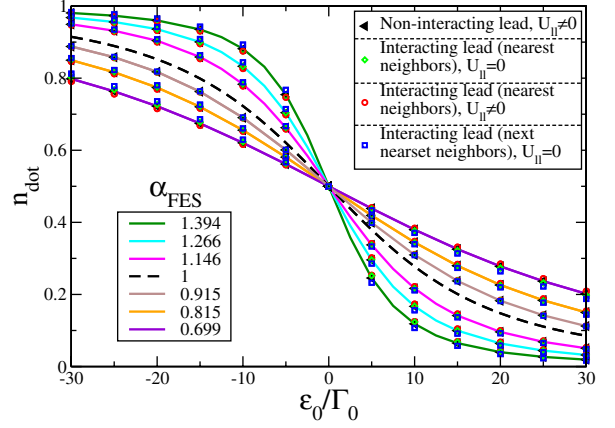


Fig. 2: (Color online) Level population as a function of its energy: different symbols denote four models used in the DMRG calculations, while the different curves (which are a guide to the eye) correspond to different α_{FES} values (the smaller α_{FES} the wider the curve and vice versa). In the last model the strengths of the nearest neighbor and next-nearest-neighbor interactions are: $\{U/t, V/t\} = \{1.5, 0.5\}$, $\{1.0, 0.5\}$, $\{0.5, 0.5\}$, $\{-0.25, -0.25\}$, $\{-0.5, -0.5\}$, $\{-0.75, -0.5\}$, in order of decreasing α_{FES} . In the third model U was taken as $\pm 0.5t$, with *opposite* sign to the corresponding fourth model case. See the text for further details.

with the term $V \sum_i (c_i^\dagger c_i - \frac{1}{2}) (c_{i+2}^\dagger c_{i+2} - \frac{1}{2})$ added to eq. (5). This is used to show that our results apply even to non-integrable models (in this system g was determined numerically). The parameters of the four models were chosen to give the same α_{FES} value (*i.e.*, in each case we have chosen arbitrarily the interactions in the lead in models c) and d), and determined by the above condition all the other interactions. The other parameters are the same as in fig. 1, except for the lead length, which is twice as large here). Again we can see that the population is universal, determined by α_{FES} alone, and not by the parameters of a specific model.

Lessons from the Kondo effect. – We now discuss another implication of the Coulomb gas mapping. The Coulomb gas we have obtained is similar to the original one, derived by Yuval and Anderson in their treatment of the anisotropic single-channel Kondo model [13]. In particular, the level population (minus one-half) in our system is equivalent to the magnetization of the Kondo impurity, the level energy ε_0 is analogous to a local magnetic field, Γ_0 plays the role of J_{\perp} , and α_{FES} is determined by J_z . We can thus immediately import all the known results from the Kondo problem [1] to the case of a LL lead coupled to a level. The system considered can be in one of two phases: a strong-coupling (antiferromagnetic Kondo like) delocalized phase, and a weak-coupling (ferromagnetic Kondo like) localized phase. At very small values of Γ_0 the transition is at $\alpha_{\text{FES}} = 2$, whereas for larger Γ_0 it occurs for larger values of α_{FES} . In the localized phase, the low-energy physics

is that of an effectively disconnected level, so that its population is discontinuous as a function of ε_0 , and there is a nonvanishing residual entropy at zero temperature. Similar results regarding this phase, as well as the phase transition line, were already discussed in ref. [5], albeit using different techniques, and tested numerically by us [9]. On the other hand, in the delocalized phase, the impurity is well hybridized with the conduction band, so the level population is analytic in ε_0 . One can write an explicit expression for this dependence using the Bethe ansatz solution of the Kondo problem [1]. In particular, for small values of ε_0 , one has

$$n(\varepsilon_0) \sim \frac{1}{2} - \frac{\varepsilon_0}{\pi T_K} \quad (8)$$

with T_K (the effective level width) corresponding to the “Kondo temperature” of the problem, which, for small Γ_0 , is given by

$$T_K = (\Gamma_0 \xi_0)^{1/(2-\alpha_{\text{FES}})} / \xi_0, \quad (9)$$

and thus reduces to Γ_0 for vanishing interactions ($\alpha_{\text{FES}}=1$). Hence, in this phase the population does not show any power law dependence on ε_0 . The only power law appearing is in the formula for T_K . However, the power depends on α_{FES} , and is nontrivial (*i.e.*, different from unity) even for a Fermi-liquid lead if level-lead interactions are not negligible, or in the presence of dissipation. The same conclusion applies to other quantities in this phase: at long time (denoted by τ) the correlation function of the level population will decay as $(\tau T_K)^{-2}$, and the entropy and specific heat will go as $1/(\beta T_K)$ for low enough temperatures. These results are in fact another manifestation of the universality property of this system: it implies that LL physics (with its ubiquitous power law dependences) *cannot* be manifested through the behavior of any of the thermodynamic properties, contrary to what one might expect based on perturbative calculations, like those performed (albeit for a different, two-lead configuration) in ref. [8] for the case $\lambda_{\parallel}=0$. Such calculations, while reproducing eq. (9), deviate from eq. (8) if g is sufficiently small.

From eqs. (8) and (9) we see that the population curve becomes wider as α_{FES} becomes smaller and vice-versa, in agreement with the numerical results shown in figs. 1 and 2. This has a simple interpretation: smaller α_{FES} corresponds, according to the previous results, to large g (*i.e.*, attraction in the lead) or positive λ_{\parallel} . Indeed, when g is larger than 1, the local density of states at the edge of a LL (or at the middle of a chiral LL) diverges at the Fermi energy [3], so tunneling is enhanced; similarly, for $\lambda_{\parallel} > 0$ tunneling is also enhanced by the Mahan exciton effect [17]: when the level is empty (full) the adjacent site of the lead tends to be full (empty) because of the charging interaction, so transition between these states becomes easier. In both cases, the population curve should indeed become broader.

Conclusions. — To conclude, we have shown that the thermodynamic properties of a level coupled to the edge of a LL are universal for a wide range of models, and are determined by only few parameters. These properties follow a single-channel Kondo physics, and thus are not qualitatively affected by the LL phase of the lead. This implies that interesting phenomena occurring in quantum impurities coupled to LLs can be studied on equivalent models with non-interacting leads, which are much easier to study, both analytically and numerically (using, *e.g.*, Wilson’s numerical renormalization group [23]). A clear signature of the LL phase can be seen when examining transport-like properties (*e.g.*, the level local density of states). Alternatively, one could extend the model to include more than one lead. Both topics will be discussed elsewhere [24].

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