Numerical study of transport through a single impurity in a spinful Tomonaga-Luttinger liquid

Yuji Hamamoto,* Ken-Ichiro Imura, and Takeo Kato
Institute for Solid State Physics, The University of Tokyo, Kashiwa, Chiba 277-8581
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The single impurity problem in a spinful Tomonaga-Luttinger liquid is studied numerically using path-integral Monte Carlo methods. The advantage of our approach is that the system allows for extensive analyses of charge and spin conductance in the non-perturbative regime. By closely examining the behavior of conductances at low temperatures, in the presence of a finite backward scattering barrier due to the impurity, we identified four distinct phases characterized by either perfect transmission or reflection of charge and spin channels. Our phase diagram for an intermediate scattering strength is consistent with the standard perturbative renormalization group (RG) analysis in the limit of weak and strong backward scattering, in the sense that all our phase boundaries interpolate the two limiting cases. Further investigations show, however, that precise location and form of our phase boundaries are not trivially explained by the standard RG analysis, e.g., some part of the phase diagram looks much similar to the weak backscattering limit, whereas some other part is clearly derived from the opposite limit. In order to give a more intuitive interpretation of such behaviors, we also reconsidered our impurity problem from the viewpoint of a quantum Brownian motion picture.

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I. INTRODUCTION

Low-energy excitations in a one-dimensional electron system are described by the so-called Tomonaga-Luttinger liquid (TLL), which is characterized by power-low decay of various correlation functions and the spin-charge separation. Recent progress in nanofabrication techniques has enabled us to realize quasi-one-dimensional quantum structures, in which TLL behaviors have been experimentally observed in, e.g., fractional quantum Hall edges and single-wall carbon nanotubes. One way to highlight such peculiar behaviors of TLL is to introduce a single impurity, which dramatically influences the transport of the system: in the low temperature limit, a conducting channel turns either perfectly transmitting or insulating.

The impurity problem in a TLL is effectively described by bosonic fields at the impurity, which is equivalent to the problem of a quantum Brownian particle moving in a periodic potential. One of the powerful ways of treating such a complicated quantum system is to numerically simulate the system using the path-integral Monte Carlo (PIMC) method. Near the phase transition, however, a simulation based on primitive local updates generally fails, and one calls for a more effective update method optimized for the system. In recent years, the efficiency of the PIMC method has been remarkably improved by the extension of the Swendsen-Wang cluster algorithm to quantum systems with continuous degrees of freedom, and the algorithm has been first applied to the phase transition in a resistance-shunted Josephson junction system.

The impurity problem in both spinless and spinful TLLs has been originally treated using perturbative renormalization group (RG) methods in the weak- and strong-impurity limits. Whether a conduction channel becomes perfectly transmitting or insulating at low temperatures is determined by the relevance of the corresponding backscattering or tunneling process. In contrast to the spinless case, in which RG analyses in the weak- and strong-backscattering limits seem to be smoothly connected, the phase diagrams of the spinful case show clear inconsistency in the two opposite limits, i.e., mismatch of RG flow, suggesting the existence of an intermediate (unstable) fixed point. Besides, the phase boundaries between conducting and insulating phases for charge and spin are expected to shift continuously as a function of the backscattering strength. Although one can see the essence of critical phenomena in this spinful system using the standard perturbative RG approach, there is little information about the phase diagram for an impurity with intermediate strength. In this paper, we adopt the effective PIMC simulations mentioned above as a non-perturbative approach to study critical phenomena in the intermediate region of impurity strength.

Our spinful impurity problem can be also understood as the physics of re-combination of the electronic charge and spin, which are generally separated and propagate with different velocities in a bulk TLL. One can introduce the scattering effect of an impurity, say, by annihilating one physical electron from the right-going mode, simultaneously creating another in the left-going mode. We mean by a physical electron, an original electron composed of both charge and spin degrees of freedom. If this scattering potential is relevant and grows stronger, the charge and spin degrees of freedom become no longer independent and their motion acquires some correlation. At low temperatures, the effect of an impurity becomes dominant. As a result the charge and spin tend to propagate almost together, realizing a situation which we call...
spin–charge re–combination, unless the difference between their bulk velocities are too large. Of course, if that difference is large enough, the charge and spin could remain nearly independent, and the spin–charge separation preserves. We will argue, based on our numerical results, whether or not the electronic charge and spin recombine depends complicatedly on the competition between the impurity strength and the difference in the original charge and spin velocities.

This paper is organized as follows. In Sec. II we state our single impurity problem in a TLL — the spinful case with intermediate backward scattering strength. In Sec. III, we give details about the path–integral quantum Monte Carlo methods employed in this work. In Sec. IV, we present our numerical results and the phase diagram deduced from our data, and then we discuss them in comparison with the known RG picture. Some further interpretation is also given in the context of quantum Brownian motion. Sec. V is devoted to the summary.

II. STATEMENT OF THE PROBLEM

Let us begin with introducing our model — the single impurity problem in a spinful Tomonaga–Luttinger liquid. Using the standard bosonization technique, we first formulate it in terms of two bosonic fields — one for charge, and the other for spin. Then, we rewrite it in a form suitable for numerical analyses. We also briefly review what is known about our model in the standard perturbative RG picture. We end this section by addressing what we will attempt to uncover throughout this paper.

A. The single impurity problem in a TLL — the spinful case

Low energy excitations of interacting one–dimensional electron system with spin are density fluctuations of charge and spin, labeled with subscripts $\rho$ and $\sigma$ respectively, and the Hamiltonian is written as

$$H_0 = \sum_{\nu = \rho, \sigma} \int \frac{dx}{4\pi} \left[ \frac{u_\nu}{K_\nu} \left( \frac{\partial \phi_\nu}{\partial x} \right)^2 + u_\nu K_\nu \left( \frac{\partial \theta_\nu}{\partial x} \right)^2 \right],$$  \hspace{1cm} (1)

where $\phi_\nu$ and $\theta_\nu$ are bosonic fields and the spatial derivative of one field is the canonical momentum of the other. $K_\rho < 1$ for repulsive interaction while $K_\sigma > 1$ for attractive, and $u_\nu$ is the sound velocity of the density fluctuation. We now consider a single symmetric impurity with finite reflection localized at the origin, and introduce backward scattering of electrons by its barrier. Using the bosonized representation of a fermionic operator $\psi_{rs}$ for an electron moving in the direction $r = R\ or\ L$ with spin $s = \uparrow$ or $\downarrow$, the Hamiltonian corresponding to the lowest order backscattering process is given by

$$H_1 = V_0 \sum_s \psi_{L,\uparrow}(0) \psi_{R,s}(0) + \text{H.c.} = v \cos \phi_\rho(0) \cos \phi_\sigma(0),$$  \hspace{1cm} (2)

Here $v$ is a parameter proportional to the scattering strength $V_0$. Note that $\phi_\nu(0)/\pi$ denotes the number of charges (spins) for $\nu = \rho(\sigma)$ in the $x > 0$ part of the system. Since the scattering term (2) influences only the fields at the origin, we can integrate out the other fields away from the barrier. If we write $\phi_\nu(\tau) \equiv \phi_\nu(x = 0, \tau)$ in the imaginary–time formalism, the effective action takes the form

$$S \equiv S_0 + S_1,$$  \hspace{1cm} (3)

$$S_0 = \sum_\nu \sum_n \frac{|\omega_n|}{2\pi K_\nu \beta} |\widehat{\phi}_\nu(\omega_n)|^2,$$  \hspace{1cm} (4)

$$S_1 = v \int_0^\beta d\tau \cos \phi_\rho(\tau) \cos \phi_\sigma(\tau),$$  \hspace{1cm} (5)

where $\widehat{\phi}_\nu(\omega_n)$ denotes the Fourier component of $\phi_\nu(\tau)$ and $\omega_n \equiv 2\pi n/\beta$ is the Matsubara frequency. $S_0$ is known as the dissipative term in the Caldeira–Leggett model,\textsuperscript{3} and can be expressed by a form of long–range interactions in $\tau$ direction as

$$S_0 = -\sum_\nu \frac{1}{2K_\nu \beta^2} \int_0^\beta d\tau \int_0^\beta d\tau' \frac{\phi_\nu(\tau) \phi_\nu(\tau')}{\sin^2 \left[ \frac{\pi}{2}(\tau - \tau') \right]},$$  \hspace{1cm} (6)

which is used when we apply the cluster algorithm to the PIMC simulation (see Sec. III).

B. Consequences of the perturbative RG, and the three–dimensional RG phase diagram in the $(K_\rho, K_\sigma, v)$–space

In order to allow for a comparison of our numerical results with the known analytic viewpoints, here we briefly review the renormalization group (RG) picture presented in Refs. 6,7. The standard perturbative RG analyses can be performed either for an infinitesimal initial value of the scattering potential $v$ in the original model (3) or in the opposite limit, i.e., for infinite backscatterings in the dual model of (3). They both give a phase diagram in the $(K_\rho, K_\sigma)$–plane characterized by four different phases, which correspond to different transport behaviors of the system in the limit $T \rightarrow 0$: (I) both charge and spin are insulating; (II) charge is conducting, while spin is insulating; (III) charge is insulating, while spin is conducting; (IV) both charge and spin are conducting. Are the phase boundaries between such four different phases dependent on the initial values of $v$? According to Refs. 6,7, the obtained phase diagram (Fig. 1) in the above two limits have, as expected, similar configurations, but the phase boundaries are not located exactly at the same position in the $(K_\rho, K_\sigma)$–plane.
Let us now ask a question, what happens if we start from an intermediate value of the scattering potential \( v \)? For such a value of \( v \), one can in principle consider a phase diagram, analogous to the above two limiting cases, i.e., probably with the same four distinct phases, but phase boundaries shifted from the two limiting cases. Since the bulk quantities \( K_\rho \) and \( K_\sigma \) are invariant under the RG transformation (because the barrier is localized at the origin), we usually focus on a straight line connecting \((K_\rho, K_\sigma, 0)\) and \((K_\rho, K_\sigma, \infty)\) for a given set of \( K_\rho \) and \( K_\sigma \), and examine how a scattering potential associated with a particular phase scales in the RG transformation. The results of Refs. 6,7 show that there exists a domain in the \((K_\rho, K_\sigma)\)-plane, in which this scattering potential is irrelevant in the limit of \( v \to 0 \), whereas relevant in the opposite limit \( v \to \infty \), indicating the existence of a non-trivial fixed point at an intermediate value of \( v \) (this fixed point is shown to be unstable). By performing the RG analyses one step further by considering higher order perturbations, one finds non-linear RG equations, suggesting a non-monotonous RG flow.

![Phase Diagram](image)

**FIG. 1:** Three-dimensional phase diagram in the \((K_\rho, K_\sigma, v)\)-space. The phase boundaries are analytically obtained in the following two limits: for a weak impurity \((v \to 0)\), the phase boundaries are three straight lines \( K_\rho + K_\sigma = 2, K_\rho = 1/2, \) and \( K_\sigma = 1/2 \); for a strong impurity \((v \to \infty)\), the phase boundaries are a hyperbola \( K_\rho^{-1} + K_\sigma^{-1} = 2 \) and two straight lines \( K_\rho = 2 \) and \( K_\sigma = 2 \). Three dotted lines represent those values of \((K_\rho, K_\sigma)\) at which phase boundaries in the \( v = 0 \) and \( v = \infty \) plane coincide.

To summarize, the standard RG approach, with the help of duality transformation, not only reveals the RG flow in the limit of weak- and strong-backscattering barriers, but, by extending the perturbative analysis one step further, it also gives us some hints about how different tendencies of RG flow in the two limits evolve and eventually merge in the region of intermediate coupling. On the other hand, there is little hope to obtain further information on the RG flow in the whole parameter space, most of which belongs to the so-called non-perturbative regime, by simply elaborating such an analytical approach. In this paper, we instead appeal to a numerical method, i.e., by performing a PIMC simulation for the effective action \( S \) given in (3), we study directly transport properties of spinful TLL with an impurity of non-perturbative backscattering potential barrier.

**III. SIMULATION METHODS**

In this section, we illustrate our numerical simulations. In order to eliminate critical slowing down at low temperature and carry out efficient simulations of the paths \( \phi_\rho(\tau) \) and \( \phi_\sigma(\tau) \), we implement local updates in Fourier space and rejection-free global updates following Refs. 10,12. Note that the single impurity problem in a spinful TLL is equivalent to the overdamped limit of the Josephson junction system discussed in Ref. 12. By discretizing the imaginary time into \( N \) time steps, we define \( \phi(j\beta/N) \) \( (j = 0, 1, \cdots, N - 1) \). Then \( S_0 \) and \( S_1 \) can be rewritten as

\[
S_0 = \sum_{v=\rho,\sigma} \sum_{k=1}^{N/2} \frac{1}{2\sigma_{vk}^2} |\tilde{\phi}_{vk}|^2, \tag{7}
\]

\[
S_1 = v\Delta T \sum_{j=0}^{N-1} \cos \phi_{\rho j} \cos \phi_{\sigma j}, \tag{8}
\]

\[
\sigma_{vk}^2 \equiv \left\{ \begin{array}{ll}
K_\rho N^2/4k & k = 1, 2, \cdots, N/2 - 1, \\
K_\rho N & k = N/2 \end{array} \right., \tag{9}
\]

where \( \Delta T = \beta/N \) and \( \tilde{\phi}_{vk} = \tilde{\phi}_{vk,N-k} = \sum_j \phi_{vj} e^{2\pi i j k} \). In a local update for \( k \neq 0 \), a new value of \( \tilde{\phi}_{vk} \) is randomly generated from a normal distribution with the variance \( \sigma_{vk}^2 \) in (9) by means of the Box-Müller method. This local update is accepted with a probability

\[
p = \min\{1, e^{-\Delta S_1}\}, \tag{10}
\]

where \( \Delta S_1 \) is the variation of the potential term (8). For the \( k = 0 \) component \( \phi_{\rho 0} \), a new value is generated from a uniform distribution ranged from \(-\pi\) to \(\pi\), and the local update is accepted again with a probability (10).

A global update scheme should be designed so that optimized paths for a given potential are efficiently generated. In the case of the double cosine potential (2), an optimized path near the phase transition typically spends most of the time in potential minima, and also has some kink structures connecting adjacent potential minima, i.e., \((\phi_\rho, \phi_\sigma) = (n_\rho \pi, n_\sigma \pi)\) with integers \(n_\rho\) and \(n_\sigma\) such that \(n_\rho \pm n_\sigma\) is odd for \(v > 0\). In order to generate such kinks, we apply the Swendsen-Wang algorithm to update of the continuous field variable \( \phi_{vj} \) following Ref. 10. To this end, we introduce a relative field variable \( \tilde{\varphi}_{vj} = \tilde{\phi}_{vj} - \phi_{vj}^{\text{mirror}} \) as shown in Fig. 2, where the reference \( \phi_{vj}^{\text{mirror}} \) is appropriately chosen as described below. If we regard the sign of the relative field \( s_{vj} = |\tilde{\varphi}_{vj}| / |\tilde{\varphi}_{vj}| \) as a spin variable, the dissipative term in (6) can be represented as a kind of one-dimensional long-range Ising
\[
S_0 = -\sum_{\nu} \sum_{j < j'} \kappa_{\nu j j'} \sigma_{\nu j} \sigma_{\nu j'}, \quad (11)
\]

where each site labeled by \( j \) corresponds to each time step \( \tau_j = j \Delta \tau \), and has two spin variables \( s_{\nu j} \) and \( s_{\nu j'} \). Due to the finite bandwidth cutoff, we should represent \( \kappa_{\nu j j'} \) as a Fourier series and restrict the sum up to a cutoff frequency as

\[
\kappa_{\nu j j'} \approx -\frac{2|\varphi_{\nu j}||\varphi_{\nu j'}|}{K_\nu N^2} \sum_{k=-N/2+1}^{N/2} |k| e^{\frac{2\pi i}{N}(j-j')k}. \quad (13)
\]

A cluster is built by connecting sites with the bond probability determined by the dissipative term \( S_0 \). In addition, the cluster is flipped with no rejection, if \( \phi_{\nu j j'}^{\text{mirror}} \) is appropriately chosen so that the potential term \( S_1 \) remains unchanged after the cluster is flipped. In Fig. 2, such rejection-free cluster updates implemented in this paper are illustrated in \( \phi_{\nu j}^{\text{mirror}} \) planes, where only the \( j \)-th path fragment in a cluster is shown.

In the upper panel (a), two mirrors are located along \( \phi_{\nu j}^{\text{mirror}} = (n_\nu + 1/2)\pi \) and \( \phi_{\nu j}^{\text{mirror}} = (n_\nu + 1/2)\pi \), where \( n_\nu \) and \( n_\sigma \) are integers. Sites are connected with bond probability

\[
p_{\nu j j'} = \max \{ 0, 1 - e^{-2\sum_{\nu} \kappa_{\nu j j'} \sigma_{\nu j} \sigma_{\nu j'}} \}, \quad (14)
\]

and both the fields \( \varphi_{\nu j} \) and \( \varphi_{\nu j'} \) in the cluster are sequentially reflected with respect to the two mirrors, i.e., \( (\varphi_{\nu j}, \varphi_{\nu j'}) \rightarrow (-\varphi_{\nu j}, -\varphi_{\nu j'}) \rightarrow (-\varphi_{\nu j}, \varphi_{\nu j'}) \). Note that the connected spins \( s_{\nu j} \) and \( s_{\nu j'} \) in one channel are not necessarily parallel, which is different from the original Swendsen-Wang algorithm. After this double-field cluster update, kink structures connecting nearest-neighbor potential minima are inserted efficiently.

Another cluster update is illustrated in the lower panel (b) in Fig. 2, where only a mirror for the charge degree of freedom is located at \( \phi_{\nu j}^{\text{mirror}} = n_\nu \pi \) with an integer \( n_\nu \). In this case, a cluster is constructed with bond probability

\[
p_{\nu j j'} = \max \{ 0, 1 - e^{-2\kappa_{\nu j j'} s_{\nu j} s_{\nu j'}} \}, \quad (15)
\]

and the relative fields \( \varphi_{\nu j} \) in the cluster are reflected with respect to the mirror, i.e., \( (\varphi_{\nu j}, \varphi_{\nu j'}) \rightarrow (-\varphi_{\nu j}, \varphi_{\nu j'}) \). A similar cluster update can be performed also for the spin degree of freedom. These single-field cluster updates insert kink structures between next-nearest-neighbor potential minima.

Using the PIMC method described above, we can efficiently simulate the impurity problem in a spinful TLL. In this paper, we observe zero-bias conductances of charge and spin channels to directly study the transport phenomena at low temperatures. In the linear response regime, a dc conductance at finite temperature is obtained from analytic continuation

\[
G_{\nu} = \lim_{i\omega_n \rightarrow 0} G_{\nu}(i\omega_n), \quad (16)
\]

where the conductance at a Matsubara frequency can be calculated from a correlation function as

\[
G_{\nu}(i\omega_n) = \frac{2e^2}{h} \frac{|\omega_n|}{\pi} \int_0^\beta d\tau \langle \phi_{\nu}(\tau) \phi_{\nu}(0) \rangle e^{i\omega_n \tau}. \quad (17)
\]

Measuring the temperature dependence of the dc conductances (16) for different sets of \( K_\nu \) and \( K_\sigma \) near the phase transition, we determine the phase boundaries in the intermediate region of the impurity strength \( v \).
K. Charge conductance $G$ and spin conductance $G_\sigma$ for different values of $K_\rho$, plotted as a function of $\omega_n$. $K_\sigma$ is fixed at $K_\sigma = 1.0$ for $N = 50, 100, 200,$ and $400$, and only the first ten points are shown for each Trotter number $N$. From top to bottom, the values of $K_\rho$ are $1.2, 1.1, 1.05, 1.025, 1.0, 0.975, 0.95, 0.9, \text{and} 0.8$. Conductance curves (of both charge and spin) show an upward bend with decreasing $\omega_n$ when $K_\rho > 1.025$, whereas they are bent downward when $K_\rho < 0.975$.

IV. RESULTS AND DISCUSSION

This section is devoted to presenting our PIMC results and the phase diagram deduced from our data. We first present and analyze our conductance curves for several given points on the $(K_\rho, K_\sigma)$-plane, and determine what kind of phase those points belong to. We then discuss the whole phase diagram, and in particular the form and the position of our phase boundaries in comparison to their counterparts in the standard perturbative RG picture (available only in the weak and strong backscattering limits). In order to uncover the nature of our phase boundaries, we also attempt to give further interpretations to them in the context of quantum Brownian motion.

A. Charge and spin conductances and their “flow” at low temperatures

We show in this subsection our simulation results for $v = 4, \Delta\tau = 0.25$, and $N = 50, 100, 200, \text{and} 400$. Here $N$ is inversely proportional to temperature as $N = \beta/\Delta\tau$.

Symmetric coupling case: $K_\rho \simeq K_\sigma$ — Let us first investigate a domain of $(K_\rho, K_\sigma)$ for which the phase diagrams in the limit of weak and strong backscattering barriers are smoothly connected. This happens when two coupling constants are symmetric, or isotropic (see Fig. 1). In Fig. 3, we focus on the $K_\sigma = 1$ line (on which the spin part is SU(2) symmetric) and plot the first ten points of $G_\rho(\omega_n)$ as a function of $\omega_n$ for different values of $K_\rho$ near the phase boundary. For a given $K_\rho$, results for different $N$, i.e., for different temperatures are superposed to form a bundle of curves. For both $G_\rho(\omega_n)$ and $G_\sigma(\omega)$, one can see that the curves for $K_\rho > 1.025$ are bent upward with decreasing $\omega_n$ (in the limit of $\omega_n \rightarrow 0$), while the curves for $K_\rho < 0.975$ are bent downward. Note also that for a given $K_\rho$, the slope of different curves composing the same bundle always becomes steeper with decreasing $\omega_n$. We will see later,
FIG. 5: (color online) Asymmetric coupling case : $K_\rho \ll K_\sigma$. Charge conductance $G_\rho(i\omega_n)$ (upper) and spin conductance $G_\sigma(i\omega_n)$ (lower) for different values of $K_\rho$, plotted as a function of $\omega_n$. $K_\sigma$ is fixed at $K_\sigma = 1.8$. $N$ = 50, 100, 200, and 400, and only the first ten points are shown for each Trotter number $N$. Charge and spin channels behave quite differently in this parameter regime. Upper : $G_\rho(i\omega_n)$ is plotted for (from top to bottom) $K_\rho = 0.600, 0.550, 0.525, 0.500, 0.475, 0.450$ and 0.400. With decreasing $\omega_n$, the charge conductance shows either a monotonic upward (first three curves) or downward (last three curves) trend. Such a behavior resembles the symmetric coupling case (see Fig. 3). Lower : $G_\sigma(i\omega_n)$ is plotted for (from top to bottom) $K_\rho = 0.500, 0.450, 0.425, 0.400, 0.375, 0.350$ and 0.300. The spin channel shows a non-monotonic behavior when $K_\rho = 0.400, 0.375$ and 0.350. For details, see also Fig. 6.

However, that the temperature dependence of $G_\sigma(i\omega_n)$ curves can become non-monotonic in the presence of a non-trivial fixed point. We have actually determined our phase boundaries by tracing the temperature dependence of dc conductances obtained from (16) following Refs 10, 12. In Fig. 4, we plot the dc conductance of charge and spin as a function of the inverse temperature $N$, which are obtained by extrapolating the first five points on each curve in Fig. 3 to $\omega_n \to 0$. With decreasing temperature, the conductances shows a monotonous increase (decrease) when $K_\rho > 1.025$ ($K_\rho < 0.975$). Here, the charge and spin channels show a simultaneous transition from conducting to insulating phase in consistent with the RG results. Recall that in the RG picture (see Fig. 1) the IV and I phases touch at $(K_\rho, K_\sigma) = (1, 1)$ both in the weak- and strong-backscattering regimes, which suggests that the phase boundary at that point is a straight line independent of $v$ in the $(K_\rho, K_\sigma, v)$-space.

Asymmetric coupling case : $K_\rho \ll K_\sigma$ — Let us turn to a parameter regime in which non-trivial RG flow is expected for a finite backscattering strength. Such a behavior is actually expected whenever the phase boundaries in the weak- and strong-impurity limits are not identical, but occurs typically when two coupling constants are highly asymmetric, or anisotropic : $K_\rho \ll K_\sigma$. In Fig. 5, we plot $G_\rho(i\omega_n)$ and $G_\sigma(i\omega_n)$ with $K_\sigma$ fixed at $K_\sigma = 1.8$, and for various values of $K_\rho$. The corresponding temperature dependence of the dc conductances is shown in Fig. 6. A careful reader might immediately notice that the charge and spin channels behave differently in these two figures. Of course, the origin of the difference is the anisotropy between $K_\rho$ and $K_\sigma$, but let us look into more carefully how they are different. In Fig. 5, conductance curves for the charge channel, i.e., $G_\rho(i\omega_n)$ with $K_\rho = 0.600, 0.550$ and 0.525 are bent upward with decreasing $\omega_n$, while the same curves for $K_\rho = 0.475, 0.450$ and 0.400 are clearly bent downward.
The temperature dependence of the dc conductance (Fig. 6) shows a monotonous behavior similar to the case of $K_v = 1$ (see Fig. 4).

On the other hand, the temperature dependence of spin conductance $G_{\sigma}(\omega_n)$ is more peculiar: for example, if one focuses on the conductance curves for $K_\rho = 0.35$, their slopes are upward at high temperatures, e.g., between $N = 50$ and 100, whereas the same curves have an opposite slope at low temperatures, e.g., between $N = 200$ and 400. Such non-monotonous behaviors might be more clearly seen, if we look into the dc conductance in Fig. 6 for $K_\rho = 0.350, 0.375$ and 0.400.

Similar crossover behaviors are observed whenever analyzing the boundary between phases I and III, and are also reported in the Josephson junction system studied in Ref. 12. From the RG viewpoint, the unusual temperature dependence of the spin channel derives from non-monotonous flows of $v$ near the intermediate unstable fixed point. Since the precise location of such a non-trivial fixed point is unknown, one cannot immediately conclude that the spin channel is in the conducting phase, even if the conductance, e.g., for $K_\rho = 0.450$ or 0.500, tends to increase monotonously toward low temperatures up to $N = 400$. Possibly, it might turn insulating at a certain lower temperature which is numerically inaccessible. Since it is difficult to locate true phase boundaries at $T = 0$ in the presence of intermediate unstable fixed points, we instead identify the phase boundary at $T \neq 0$ by observing the temperature dependence near the lowest temperature $N \approx 400$.

B. The phase diagram in the $(K_\rho, K_\sigma)$-plane for an intermediate scattering strength

Repeating the analyses outlined in the previous subsection for different sets of $K_\rho$ and $K_\sigma$ near the phase transition, we determine the whole phase boundaries in the $(K_\rho, K_\sigma)$-plane. In Fig. 7, we show our phase diagram for a finite impurity strength $v = 4$ obtained from the PIMC simulations at inverse temperature $\beta = 400\Delta\tau$. Due to the symmetry of the action (3) in terms of $\rho$ and $\sigma$, the following discussion also holds true when the charge and spin degrees of freedom are interchanged. In that case, the phases II and III are, of course, exchanged.

In Fig. 7 one can see three different phases: (Phase I) neither charge nor spin is conducting, (Phase III) only spin is conducting, (Phase IV) both charge and spin are conducting. The phase boundaries are shown by solid lines. If one compares them with the phase boundaries obtained by the renormalization group (RG) analyses in the weak and strong backscattering limits, one can verify that all the boundaries are indeed located between the two limiting cases. However, the way they are shifted from either of the limits is not uniform, i.e., for nearly isotropic interactions $K_\rho \approx K_\sigma$, our phase boundary at an intermediate coupling is much closer to the weak backscattering (WBS) phase boundary, whereas for strongly anisotropic interactions $K_\rho \ll K_\sigma$, our phase boundary between I and III phases is much closer to the strong backscattering (SBS) phase boundary. Similarly, our III-IV boundary is much closer to the WBS boundary. Correspondingly, the tricritical point, i.e., the meeting point of I, III, and IV phases, lies between its counterparts in the WBS and SBS limits.

For nearly isotropic interactions $K_\rho \approx K_\sigma$, the obtained critical lines for a finite $v$ between insulating (I) and conducting (IV) phases looks much similar to the WBS boundary: $K_\rho + K_\sigma = 2$. This can be understood as a result of the large conductances of the charge and spin channels (see, e.g., Fig. 4). Then, we can judge that our scattering potential $v$ is relatively small. For strongly anisotropic interactions $K_\rho \ll K_\sigma$, the III-IV boundary also resembles its WBS counterpart: $K_\rho = 1/2$, while the I-III boundary does not. Interestingly enough, for a broad range of $K_\rho$, say, $0 < K_\rho < 0.3$, the latter boundary is almost superposed on the SBS phase boundary: $K_\sigma = 2$, which contradicts a naive expectation from the presumably small scattering potential. Thus increasing anisotropy, the position of our phase boundary shifts from that of WBS to SBS counterparts.

In order to clarify such rather unexpected behavior of the I-III boundary, here we discuss how vertical and horizontal boundaries appear in the $(K_\rho, K_\sigma)$-plane. As an example of these boundaries, let us recall the RG phase diagram in the WBS and SBS limits in Fig. 1. In the WBS case, a vertical boundary appears between III-IV ...
phases, where the interactions are strongly anisotropic ($K_{\sigma} \ll K_{\rho}$) and, for $K_{\sigma} > 2$, the phase diagram is characterized only by the value of $K_{\rho}$. Due to the strong attraction $K_{\sigma} \gg 1$, the spin channel transmits through the impurity so freely that the weak scattering potential hardly influences this spin channel. In that sense, the spin mode is irrelevant and the transport of the system depends only on the charge mode, which we call a one-field situation. In the SBS case, on the other hand, a horizontal boundary appears between I-III phases, where again the interactions are fully anisotropic and, for $K_{\sigma} < 1/2$, the phase diagram is characterized only by the value of $K_{\sigma}$. Due to the strong repulsion $K_{\rho} \ll 1$, the charge channel scarcely go over the impurity, and is almost extinct. Then again, we see another one-field situation. In both the WBS and SBS cases, the vertical or horizontal boundary appears as a result of the strong anisotropy in the interactions, rather than the extreme values of $v$.

We can now interpret the unexpected change of the I-III phase boundary observed in Fig. 7. The horizontal region in the I-III boundary derives from the occurrence of a one-field situation where transport of the system is characterized only by the spin channel. Thus, after integrating out the extinct charge channel, one can argue that the effective action is given by

$$S \simeq \sum_{\omega_n} \frac{|\omega_n|}{2\pi K_{\sigma}} |\phi_\sigma(\omega_n)|^2 + v \int d\tau \cos \phi_\sigma(\tau),$$

(18)

which takes the same form as the action of a single impurity problem in a spinless TLL with interaction parameter $K = K_{\sigma}/2$. Our phase diagram implies that the I-III boundary in the SBS limit: $K_{\sigma} = 2$, partially preserves its position for a broad range of $v > 0$, leading to the robustness of the boundary. The I-III boundary in Fig. 7 also shows a small deviation from $K_{\sigma} = 2$ with increasing the value of $K_{\rho}$. In this parameter region, the pinning of charge degree of freedom is no longer complete, and we believe that the crossover from the one-field model (18) to the original two-field model (3) occurs. We will give further discussion on this behavior in the context of quantum Brownian motion in the next subsection. Note that, due to the duality of the impurity problem in a TLL, the III-IV boundary will also show a similar crossover for a large value of $v$.

It should also be added that a model qualitatively equivalent to the single impurity problem in a spinful TLL is realized in a completely different context. Werner et al. have performed the PIMC simulations of a system with two Josephson junctions, and shown a phase diagram similar to Fig. 7 consisting of three distinct phases. Although the kinetic term derived from charging energy $E_C$, which is absent in our model, does not change the essential nature of the phase boundaries, it nevertheless influences transport phenomena at low temperatures. In Ref. 12, the authors seem to assume that the system undergoes transition to a one-field model like (18) as soon as a channel enters an insulating phase, and that the position of the tricritical point is independent of the Josephson coupling strength $E_J$, which corresponds to the backscattering strength $v$ in our system. As we have seen above, however, the original two-field model slowly crossovers to a one-field one, and so the tricritical point should in general depend on $E_J$, or $v$. If our conjecture holds true also for the two-Josephson-junction system, the discrepancy in the tricritical point discussed in Ref. 12 would be resolved.

**C. Interpretation in the context of quantum Brownian motion**

In the previous subsections, we have seen the system not only undergoes transition between insulating and conduction for charge and spin channels, but also crossovers from the original two-field (3) to a one-field model like (18). In order to interpret the crossover more clearly, let us reconsider our previous results from the viewpoint of quantum Brownian motion. As is clear from the Caldeira-Leggett form of the action (3), our spinful single barrier problem is equivalent to two-dimensional dynamics of a massless quantum Brownian particle in a periodic potential. In this picture, the bosonic fields ($\phi_\rho, \phi_\sigma$) play the role of particle’s coordinates. As shown in Fig. 8, the potential $v \cos \phi_\rho \cos \phi_\sigma$, for $v > 0$, has minima (maxima) at $(n_\rho \pi, n_\sigma \pi)$ with integral $n_\rho$ and $n_\sigma$ such that $n_\rho + n_\sigma = odd\ (even)$. Each minimum corresponds to a certain ground state where integral numbers of electronic charges and spins exist in the $x > 0$ part of the system. The dissipation strengths in the $\phi_\rho (\phi_\sigma)$ direction is proportional to $K_{\rho}^{-1} (K_{\sigma}^{-1})$.

For nearly isotropic dissipations $K_{\rho}^{-1} \simeq K_{\sigma}^{-1}$, the particle at low temperatures tunnels from one minimum to another, usually through a saddle point between them, and only occasionally over a maximum. Although charge
and spin are generally separated and propagate with different velocities in a TLL, tunneling through a saddle point recovers the spin-charge combined nature of a physical electron. On the other hand, for strongly anisotropic dissipations, e.g., $K^{-1}_{\rho} \gg K^{-1}_{\sigma}$, the position of the most relevant tunneling process could be taken by the other.

If the friction in the $\phi_{\rho}$ direction is large enough to suppress completely the tunneling through a saddle point, the particle can only go over a potential maximum in the $\phi_{\rho}$ direction toward another minimum. In this case, the system is dominated by the one-dimensional action (18) describing the horizontal part of I-III boundary in Fig. 7. If the friction in the $\phi_{\sigma}$ direction is so small that the massless particle can move freely in that direction, the system depends only on the $\phi_{\rho}$ coordinate and one gets another one-dimensional action analogous to (18).

If we now return to the original TLL picture, the crossover from a two-field to a one-field model depends on the anisotropy of interactions and the impurity strength $v$ in a complicated way. Moreover, the phase diagram in Fig. 7 shows a crossover behavior in the $K_{\rho}-K_{\sigma}$ plane for an intermediate anisotropy, where the effective action can no longer be written in such a simple form as (18). It is worth noting that in the small- and large-barrier limits, crossovers to a one-field model occurs in so small a region that one cannot observe them in the phase diagram in Fig. 1, while the PIMC simulation does demonstrate that they could actually appear in a broad range of $v$.

V. SUMMARY

In this paper, we have studied the single impurity problem in a spinful TLL using the path-integral Monte Carlo methods. Measuring the temperature dependence of the charge and spin conductances, we have obtained the phase diagram characterized by perfect conduction or insulation of the charge and spin channels, which is consistent with the renormalization group (RG) results in the weak- and strong-impurity limits. We have also observed non-monotonous temperature dependence of conductances, which qualitatively supports the non-linear flows near non-trivial unstable fixed points predicted in the RG picture. The phase diagram obtained from our simulations for an impurity with intermediate strength shows unexpected shift of a phase boundary for strongly anisotropic interactions. By mapping the impurity problem to a quantum Brownian motion picture, we have proposed an intuitive interpretation of this behavior from the viewpoint of crossover to a one-field model.

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