Continuous-Time Quantum Monte Carlo Study
of Local Non-Fermi Liquid State in the Multichannel Anderson Model

Junya Otsuki

Department of Physics, Tohoku University, Sendai 980-8578

The impurity Green’s function $G_f$ in the local non-Fermi liquid state is evaluated by means of the continuous-time quantum Monte Carlo method extended to the multichannel Anderson model. For $N = M$ (where $N$ and $M$ are numbers of spin components and channels, respectively), $G_f$ is expressed as $-\text{Im}G_f(\omega + i0) = c - b|\omega|^{1/2}$, and the zero-frequency value $c$ depends only on $N (= M)$. A corresponding impurity self-energy at low frequencies is composed of two parts: a resonance term related to $c$, and a non-Fermi liquid term proportional to $|\omega|^{1/2}$. The characteristic energy scale is discussed in terms of the non-Fermi liquid term in the self-energy.

KEYWORDS: continuous-time quantum Monte Carlo (CT-QMC), two-channel Kondo effect

1. Introduction

The multichannel Kondo effect is a typical example that leads to a local non-Fermi liquid ground state.\(^{3,4,5}\) It has been recognized that the peculiar low-temperature behaviors observed in uranium compounds and metals with uranium impurities are due to the two-channel Kondo effect.\(^{2,3}\) This kind of non-Fermi liquid state has been investigated from a dynamical point of view based on models generalized to SU($N$) $\otimes$ SU($M$) symmetry.\(^{3,5}\) Then, their critical nature has been discussed extensively.\(^{3,8}\)

Regarding the (single-channel) Kondo problem, the Anderson Hamiltonian gives clear insight:\(^{6,7}\) the ground state is connected to that in the non-interacting limit. In this analogy, the multichannel Kondo effect can be addressed based on an Anderson Hamiltonian.\(^{3,5}\) The inclusion of the impurity charge degree of freedom enables us to describe the local dynamics via the impurity Green’s function. We thus consider the SU($N$) $\otimes$ SU($M$) multichannel Anderson model given by\(^{2}\)

$$\mathcal{H} = \sum_{\alpha, \mu} \varepsilon_{\alpha} c_{\alpha \mu}^\dagger c_{\alpha \mu} + E_{\text{ex}} \sum_{\alpha} X_{\alpha, \alpha}$$

$$+ V \sum_{\alpha, \mu} (X_{\mu}, - \alpha) c_{\alpha \mu} + \text{h.c.}. \quad (1)$$

The (pseudo-)spin index $\mu$ and channel index $\alpha$ run over $N$ and $M$ components, respectively. The $f^2$ state $|\mu\rangle$ forms a channel singlet ($-\alpha$ denotes the counterpart of $\alpha$), and the $f^1$ state $|\alpha\rangle$ has the energy $E_{\text{ex}}$ relative to $|\mu\rangle$. The Hilbert space of $f$ states is restricted to $|\alpha\rangle$ and $|\mu\rangle$ by using the $X$-operators $X_{\gamma, \gamma'} = \langle \gamma | \gamma' \rangle$ with $\gamma = \alpha, \mu$, on which $\sum_{\gamma} X_{\gamma, \gamma} = 1$ is imposed. $c_{\alpha \mu} = N_0^{-1/2} \sum_k c_{\alpha \mu k}$ with $N_0$ being number of sites. The $M$-channel Coqblin-Schrieffer model is derived from the Hamiltonian (1) as a localized limit $V^2$, $E_{\text{ex}} \to \infty$ with $V^2/E_{\text{ex}}$ fixed. Exact thermodynamics of the model (1)\(^{9}\) as well as the localized limit\(^{10}\) has been derived.

Concerning the dynamical properties, a two-channel case, $N = M = 2$, has been clarified by the numerical renormalization group\(^{10}\) and by an exact method.\(^{11}\) General cases have been investigated by perturbational treatments.\(^{3,12,13}\) In this paper, we numerically investigate the dynamical properties of the multichannel Anderson model. To this end, we develop an algorithm based on the recently developed continuous-time quantum Monte Carlo (CT-QMC) method,\(^{14-16}\) which is explained in the next section. We show numerical results for the impurity Green’s function and self-energy in §3.

2. CT-QMC for the multichannel Anderson model

We study the model (1) by the CT-QMC, which evaluates a perturbation expansion stochastically. In the present case, we adopt the hybridization expansion.\(^{15}\) Since the non-perturbative part is diagonal with respect to $\alpha$ and $\mu$, the efficient algorithm using a ‘segment’ picture is applicable by a slight modification. Figure 1 shows a diagram of a configuration of order $V^6$. Spin states $\mu_i$ and channel states $\alpha_i$ appear alternately, which are hereafter referred to as segment and anti-segment, respectively. In general, a configuration of order $V^{2k}$ is represented by $q_k \equiv \{\tau_i, \alpha_i, \tau_i, \alpha_i\}$. The trace over the local states is thus taken into account graphically. On the other hand, the trace over conduction electrons is evaluated based on Wick’s theorem. A Monte Carlo sampling is performed in the configuration space composed of $k$ and $q_k$.

We perform the following update processes: (i) addition/removal of a segment or an anti-segment, and (ii) exchange of spin or channel indices. Fig. 2(a) shows the addition of a segment. The index $\mu$ of the segment is randomly chosen, and accordingly the update probability differs from that in ref. 15 by a factor of $N$. When either $N$ or $M$ is larger than 2, the ergodicity is not satisfied only by process (i). For

![Fig. 1. Diagrammatic representation of a configuration of order $V^6$. The outgoing and incoming allows indicate creation and annihilation of conduction electrons, respectively.](image-url)
example, configurations shown in Fig. 3 cannot be reached. This problem can be solved by introducing a process shown in Fig. 2(b), which exchanges the spin indices. We perform a similar update to exchange the channel indices as well.

In the simulation, we observe negative weight configurations for $N = M > 2$. However, since their contribution is less than 10% in the parameter range shown in this paper, the sign problem has little effect on the simulation.

3. Numerical Results

In this paper, we restrict ourselves to $N = M$. We use a rectangular density of states $ρ(ε) = (1/2D)θ(D − |ε|)$ for conduction electrons with $D = 1$. We fix $NV^2 = 0.12$ so that the exponent of the Kondo temperature is the same for different $N$. The width of the localized state $Δ = πV^2ρ(0)$ is $Δ ≃ 0.094$ at most (for $N = 2$), and therefore the effect of finite band width may be neglected.

3.1 Green’s function

We first show results for the single-particle Green’s function $G_f$, which is defined in the restricted Hilbert space by

$$G_f(ie_n) = −∫_0^β dτ(X_{−α,μ}(τ)X_{μ,−α})e^{iε_nτ},$$  \hspace{1cm} (2)

where $ε_n = (2n + 1)πT$ is the fermionic Matsubara frequency. At high frequencies, $G_f$ follows $G_f(ie_n) ∼ a/ε_n$ with $a < 1$, since the Hilbert space is restricted. The $a$ varies between $1/N$ and $1/M$ depending on $E_{ex}$, and in a special case of $N = M, a = 1/N$.

In Fig. 4, $−ImG_f(ie_n)Δ$ is plotted against $ε_n$ for $E_{ex} = 0$. For all $N = M, G_f$ is expressed as $−ImG_f(ie_n) = c − b/|ε_n|^{1/2}$ at low frequencies. Hence, $G_f(z)$ is non-analytic at $z → +i0$, and the spectrum $−ImG_f(ω + i0)$ on real frequencies exhibits a cusp structure expressed by $c − b/|ω|^{1/2}$, which has been reported for $N = M = 2, 4, 10, 11$. The value $c$ at $ε_n → +0$ decreases with increasing $N$. From Fig. 4 and an analogy with the Friedel sum-rule in the Fermi liquid, we conjecture the following relation:

$$−ImG_f(±i0) = \frac{1}{Δ} sin^2 \left(\frac{π}{2N}\right).$$  \hspace{1cm} (3)



Fig. 2. Update processes: (a) addition of a segment, and (b) exchange of spin indices.

Fig. 3. Examples of diagrams which cannot be reached without the ‘exchange’ process. The spin and channel components are labeled as 1, 2, · · · , and $a, b, · · ·$, respectively.

Fig. 4. (Color online) The imaginary part of the Green’s function $G_f(ie_n)$ for $N = M, NV^2 = 0.12, E_{ex} = 0$ and $T = 0.0001$. The lines show $sin^2(π/2N)$.
3.3 Effect of Level Splitting

So far, we have examined $E_{\text{ex}} = 0$. We now discuss the effect of $E_{\text{ex}}$. In refs. 10 and 11, it is reported for $N = M = 2$ that $\text{Im} G_f (+i0)$ and $\text{Im} \Sigma_f (+i0)$ do not depend on $E_{\text{ex}}$. We have confirmed for $N = M \geq 2$ that eqs. (3) and (8) hold up to $E_{\text{ex}} = 0.3$ within numerical accuracy. The finite value of $E_{\text{ex}}$ causes an asymmetry of the cusp keeping the value at $\omega = 0$: $c + b(|\omega|^{1/2})$ changes into $c + [b_{+} \theta(\omega) + b_{-} \theta(-\omega)]|\omega|^{1/2}$.

As $E_{\text{ex}}$ increases, the energy scale becomes smaller.

define a characteristic energy scale $T_0$ in terms of $\tilde{S}_f$ by

$$-\text{Im} \tilde{S}_f (i\epsilon_n)/a\Delta \sim (\epsilon_n/T_0)^{1/2},$$

in the limit $\epsilon_n \to 0$. Because $T_0$ may be defined with an arbitrary factor, we shall discuss only its exponent. In Fig. 6, we show $T_0$ as a function of $E_{\text{ex}}$. $T_0$ follows $T_0 \propto T_K \propto \exp(-1/g)$ with $g = NV^2\rho(0)/E_{\text{ex}}$ for $E_{\text{ex}} \gtrsim 0.15$, namely $g \lesssim 0.4$. We conclude that the exponent of the energy scale of the non-Fermi liquid self-energy agrees with the Kondo temperature $T_K$ in the corresponding single-channel model.

4. Summary

We have presented the impurity Green’s function $G_f (i\epsilon_n)$ and the self-energy $\Sigma_f (i\epsilon_n)$ in the non-Fermi liquid state using the CT-QMC extended to the multichannel Anderson model. For $N = M$, $G_f$ and $\Sigma_f$ are non-analytic at $\omega = 0$ as $|\omega|^{1/2}$. The zero-frequency spectrum $\text{Im} G_f (+i0)$ does not depend on the excitation energy $E_{\text{ex}}$, and consequently $\text{Im} \Sigma_f (+i0)$ has a finite value. These values depend only on $N (= M)$, and seem to be expressed as eqs. (3), (7) and (8). An analysis of general $N, M$ is left for future work.

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