CT-QMC and Maximum Entropy Approach to a Scattering-States Formulation of Strongly Correlated Steady-State Transport

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Abstract. In a recent work [17] Han and Heary introduced a formalism approaching steady-state quantum transport through mesoscopic structures which maps the non-equilibrium problem onto a family of auxiliary equilibrium quantum impurity systems by introducing imaginary voltages. We apply continuous-time quantum Monte-Carlo solvers to obtain precise and unbiased imaginary-time data for these auxiliary models. Physical observables are obtained by an analytical continuation in both Matsubara frequency and complexified voltage using a Maximum Entropy Method (MEM). The MEM is introduced by means of a kernel function compatible with the analytical structure of the theory. While it remains a yet challenging task to obtain reliable spectral functions, this unbiased procedure seems to indicate that the formalism yields results which are compatible with those of other methods.

1. Introduction
Calculating steady-state transport properties of open quantum systems is a challenging and unsolved problem. It has been approached by perturbative methods [1–3], the time-dependent density matrix renormalization group (t-DMRG) [4, 5], real-time quantum Monte Carlo (RT-QMC) [6–9], numerical renormalization group (NRG) [10], and the functional renormalization group (fRG) [11–16]. However, none of the methods developed so far is able to give a complete and reliable description of the physical properties in all parameter regimes. More importantly, the most interesting regime, where all relevant energy scales – voltage, temperature, magnetic field, etc. – are of the same order as the low-energy scale of the Anderson Impurity Model, is usually not accessible. Therefore, the development of new or improved simulation approaches is a worthwhile and important task.

Recently, a new and rather unconventional approach to calculate the steady-state transport through interacting quantum dots or similar structures was proposed by Han and Heary [17]. Their formalism, which is based on Hershfield’s density operator [18], maps the non-equilibrium steady-state of the interacting model onto an infinite set of auxiliary equilibrium systems, each characterized by some complex voltage. The complexification of the voltage bias, however, introduces a formidable new problem in the form of an analytical continuation with respect to
the voltage on top of the already challenging analytic continuation from Matsubara frequencies to real frequencies.

In a recent preprint [19] we applied Continuous-Time Quantum Monte Carlo [20–22] in order to obtain high-quality data and proposed a scheme for analytical continuation using a Maximum Entropy Method [23, 24]. For the latter purpose, a linear integral equation was derived. We review the results and introduce a possible generalization of the approach.

2. Physical Model and Imaginary Voltages

We consider the single-impurity Anderson model attached to two Fermi liquid leads,

\[ H = \sum_{\alpha k \sigma} \varepsilon_{\alpha k} c_{\alpha k \sigma}^\dagger c_{\alpha k \sigma} + \sum_{\sigma} V_G d_{\sigma}^\dagger d_{\sigma} + \sum_{\alpha k \sigma} (V_{\alpha k} c_{\alpha k \sigma}^\dagger d_{\sigma} + V_{\alpha k}^* d_{\sigma}^\dagger c_{\alpha k \sigma}) + U \left( n_{\uparrow} - \frac{1}{2} \right) \left( n_{\downarrow} - \frac{1}{2} \right), \]

where \( V_G \) is the gate voltage, \( U \) is the Coulomb repulsion, \( V_{\alpha k} \) the hybridization between quantum dot and lead and \( \varepsilon_{\alpha k} \) are the dispersion relations of the left (\( \alpha = -1 \)) and right (\( \alpha = +1 \)) leads. The two leads have temperature \( \beta \) and different chemical potentials \( \mu_{\alpha} \), with the bias voltage \( \mu_L - \mu_R = \Phi \).

In the formalism by Han and Heary, the resulting non-equilibrium steady-state problem is mapped to the equilibrium quantum impurity problems given by the effective action for the dot electrons,

\[ S_{\text{eff}} = \sum_{\sigma} \int_0^{\beta} d\tau' d\tau \left( \sigma G_{0\sigma}(\tau', \tau) d_{\sigma}(\tau) + U \int_0^{\beta} d\tau' \left( d_{\uparrow}(\tau') d_{\downarrow}(\tau) - \frac{1}{2} \right) \left( d_{\downarrow}(\tau') d_{\uparrow}(\tau) - \frac{1}{2} \right) \right), \]

where the bare Green’s function \( G_0(i\varphi_m, i\omega_n) = \sum_{\alpha=\pm1} \frac{\Gamma_{\alpha}/\Gamma}{\omega_n - V_G - \frac{1}{2}(i\varphi_m - \Phi) + i\pi\text{sgn}(\omega_n - \alpha\varphi_m)/2} \)

depends on the imaginary voltages \( \varphi_m = \frac{4\pi m}{\beta} \), \( m \in \mathbb{Z} \) which parametrize the set of equilibrium systems.

The action is solved using continuous-time QMC solvers [20–22]. Typical Monte-Carlo results from the interaction expansion solver are shown in the left panel of Fig. 1. High quality data (error bars of the order of the linewidth) are obtained for the non-trivial regime.
Figure 2. Analytic Structure. Green crosses (circles) denote QMC data which are (are not) taken into account.

$$\Phi \approx V_G \approx \beta^{-1} \approx T_K$$, where $T_K$ is the equilibrium Kondo temperature. Analytical continuation of the data at $\Phi = 0$ yields a good agreement with results obtained from equilibrium QMC data for conventional Matsubara theory and the conventional Wick rotation inferred by a Maximum entropy method for the integral representation $G(i\omega_n) = \int d\varepsilon A(\varepsilon) e^{i\omega_n \varepsilon}$. This is shown in the second panel of Fig. 1.

3. Analytic Continuation Procedure
The analytic continuation procedure we used [19] can be summarized as follows. The complexified Green’s function $G(i\varphi_m \rightarrow z_\varphi, i\omega_n \rightarrow z_\omega)$ has branch cuts for certain ratios of the imaginary parts of the complex variables. Those branch cuts are denoted by lines in the left panel of Fig. 2 and occur for ratios $\text{Im } z_\omega = \frac{\gamma}{2} \text{Im } z_\varphi$, $\gamma$ odd. The desired limiting procedure for the analytic continuation is denoted by the dash-dotted arrow. Hence, the data points within the cone $C_\varepsilon$ are considered, where the branch cut $\gamma_{\text{crit}}$ is the last relevant branch cut. This is because the series of relevant branch cuts is expected to terminate at a finite $|\gamma_{\text{crit}}| < \infty$ at finite temperature and interaction. [17] Using analyticity with respect to two complex variables within the domain $T^{C_\varepsilon} = \mathbb{R}^2 + iC_\varepsilon$ the following integral representation with respect to the edge of the domain can be derived [19]:

$$\text{Im } G(\bar{z})|_{T^{C_\varepsilon}} = -\pi \int_{\mathbb{R}^2} d^2x \, P_\varepsilon(\bar{z} - x) \tilde{A}(x),$$  \hfill (2)

with

$$P_\varepsilon(z) = \frac{2}{\pi^2 \varepsilon} \prod_{\mu = \pm 1} \frac{y_2 - \mu y_1/\varepsilon}{(x_2 - \mu x_1/\varepsilon)^2 + (y_2 - \mu y_1/\varepsilon)^2}. \hfill (3)$$

The function $\tilde{A}(x)$ is inferred via the Maximum Entropy Method, and the dot electron spectral function is then given by $A(\omega) = \tilde{A}(\Phi, \omega)$. Data in the right panel of figure 1 were calculated with this procedure.

4. Extension of the Procedure
Experience, however, shows that the exclusion of QMC data in the other cones is suboptimal from a stochastic point of view. In the right panel of figure 2 an arbitrary cone is considered, for
which the Green’s function is holomorphic. We find that a crucial property of the two-variable Green’s function, namely the shared real part at the point were the branch cuts cross, suffices to connect the analytic properties of all cones. This property may easily be verified for the bare Green’s function. For the interacting case a rigorous proof is still missing. It may, however be motivated by an argument based on hermiticity.

We use the generalization of conformal transformations to several complex variables, called biholomorphic transformations, to perform the generalization. Namely, the formal rotation of a cone to a cone ("reconstruction cone"), for which the Kramers-Kronig relation with respect to one complex variable may be applied, is such a transformation. We define the Hilbert transformation \( Hf(x, y) = \frac{1}{\pi} P \int_{-\infty}^{\infty} \frac{f(\tilde{x}, \tilde{y})}{y - \tilde{y}} \, d\tilde{y} \). and the rotation operator \( R_\vartheta \) which maps a function located on a cone to the cone rotated by angle \( \vartheta \) using a coordinate transformation.

A straightforward calculation yields data not contained in the \( C_\epsilon \)-cone may be related to the spectral function in a linear fashion in the following way:

\[
\text{Im} G|_{TC_\vartheta} = \pi \cdot P_\epsilon, \vartheta \cdot H \cdot \hat{A} =: K_\epsilon, \vartheta \cdot \hat{A}.
\]

Here,

\[
P_\epsilon, \vartheta ((i \varphi_m, i \omega_n)^T - \vec{x}) = P_\epsilon (R_\vartheta^{-1} ((i \varphi_m, i \omega_n)^T - \vec{x})),
\]

with the rotation matrix \( R_\vartheta^{-1} = \begin{pmatrix} \cos \vartheta & -\sin \vartheta \\ \sin \vartheta & \cos \vartheta \end{pmatrix} \). Current efforts focus on implementing this relation into the Maximum Entropy procedure in order to improve the quality of the inferred solutions.

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