Determination of the Many-Body Conductance of a Fully Interacting System of Electrons

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Abstract

New simulation tools are required to correctly capture the physics of strongly interacting systems. Here, we present results of a new technique for extracting the many-body conductance for interacting systems in two or three dimensions. Our approach is to extend many-body path integral Monte Carlo (PIMC) simulations, which we have used for small quantum dots [1], to much larger, two-dimensional, simulations of several different quantum point contact (QPC). In each QPC, we simulate up to two hundred fully interacting electrons in a fully quantum many-body framework. This technique allows the seamless simulation of both the dense 2DEG in the contacts and a low-density, quasi-1D correlated electron distribution in the device, as illustrated in Fig. 1.

Estimating the Conductance

To estimate the DC conductance, we collect the current-current correlation function, which we measure in imaginary time (illustrated in Fig. 2),

$$\Pi(x,x';i\tau)=\langle j_x(x;0)j_x(x';i\tau)\rangle_\beta \qquad (1)$$

The Fourier transform is a set of real amplitudes at the bosonic Matsubara frequencies, $\omega_n=\frac{2n\pi}{\beta}$,

$$\Pi(x,x';i\omega_n)=\sum_{m=0}^{\infty}e^{i\omega_n m\tau}\,\Pi(x,x';im\tau)\tau \qquad (2)$$

The conductivity is then given by the Kubo formula,

$$\sigma(x,x';\omega)=\frac{i}{\omega}\left[\Pi(x,x';\omega)+\frac{ne^2}{m}\right] \qquad (3)$$

To obtain $\Pi(x,x';\omega)$ requires analytic continuation from the Matsubara frequencies, formally denoted as $i\omega_n\to\omega+i\delta$. The $i\delta$ part of the notation dictates that for the retarded Green's functions, the real frequency axis must be approached in the upper-half plane. Therefore, we must use the collected data for the Matsubara frequencies in the upper-half plane and analytically continue them to small real-valued frequencies. Once the conductivity is then fit to a Drude formula based model and the DC conductance is extracted.

QPC with Several Hundred Electrons

Here we take a simple analytic expression [2] for a split-gate QPC that is 200 nm in length and 50 nm in width containing 200 total electrons (100 spin up and 100 spin down). We obtain the current-current correlation functions, as described in the previous section, as well as the electron density and correlation functions. In Fig. 3, we plot the conductivity at the first Matsubara frequency for V_g = -0.3 V. We find that it is essentially diagonal and that the conductivity is suppressed within the channel and that the transport is purely local in nature. In Fig. 4, we plot the DC conductance for V_g = -0.3 V. We solve for the conductance in the steady-state limit using an N-point Padé approximation. Here we see that the conductance is also suppressed in the channel corresponding to the high negative gate bias. While the conductance is low, the conductance is still higher than in the case of the non-interacting electrons as the interactions force the electrons to higher energies.

Further, we will show that our new method yields the same conductance values as that of Green's functions in the non-interacting system and analyze the resultant Kondo behavior near pinch-off.

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[1] M. Harowitz, D. Shin, and J. Shumway, J. of Low Temp. Phys. **140**, 211-226 (2005).
[2] G. Timp, Semicond. and Semimetals **35**, 113 (1992).

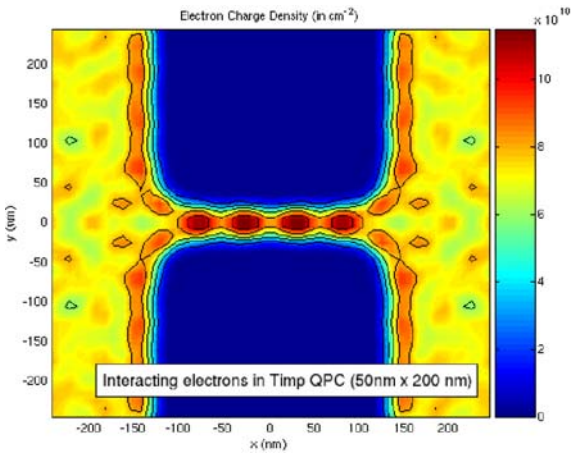

Fig. 1. Example of charge density in and around a model QPC, as calculated with our new many-body PIMC technique. The method seamlessly includes both the dense 2DEG outside the channel and the highly-correlated, quasi-1D electron ordering within the device.

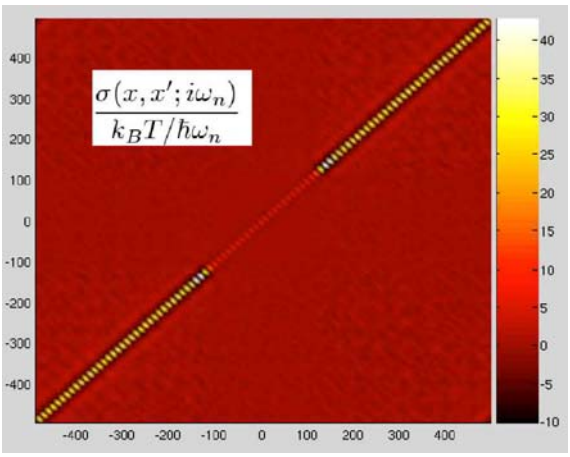

Fig. 3. The conductivity at the first Matsubara frequency, as calculated by sampling the current-current correlation function for 200 interacting electrons at V_g = -0.3 V. The device is in the range -100 nm < x < 100 nm and is coupled to wide leads, which display much higher conductivity.

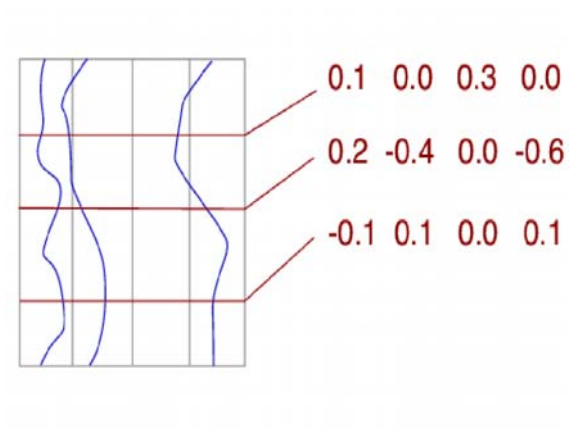

Fig. 2. A schematic illustration of collecting charge current density information from the PIMC. We set up discrete real-space bins, then histogram the location and velocities of discretized beads. We then use an FFT to convolve the data for the relative time separations and collect the current-current correlation functions over many path configurations.

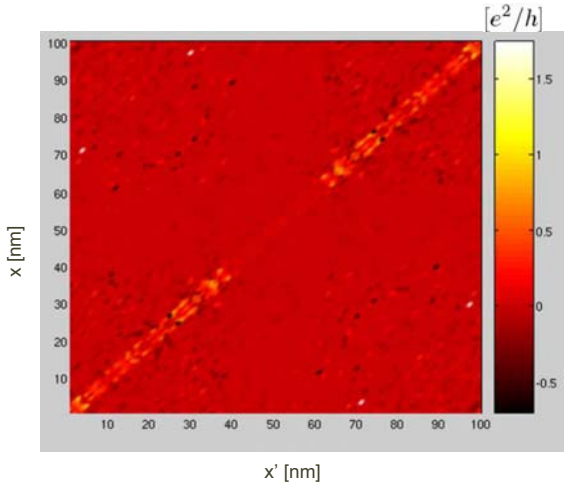

Fig. 4. DC conductivity as extrapolated using an N-point Padé approximation at V_g = -0.3 V. While the conductance is quite clear, the off-diagonal values represent statistical noise in our simulation which may be reduced with longer Monte Carlo runs.