Reply to "Comment on: Magnetotransport through graphene spin valves and its following works"

by Y. Zhou and M.W. Wu

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Abstract

In their comment Y. Zhou and M.W. Wu claim that the fundamental transport equation relating the current to the transmission function, used by us and in fact by numerous other researchers, is invalid for extended systems and should be corrected. They provide a "correct" new formula for transport in extended systems. This would be indeed a surprising new aspect of quantum transport theory. Here we show mathematically, however, that the "new formula" is a misconception resulting from adding an energy and momentum dependent function that has to vanish, due to fundamental reasons. Results and conclusions stemming from adding this function are irrelevant. The known established formulas for quantum transport are consistent with each others under the well-documented conditions.
In their comment [1] Y. Zhou and M.W. Wu argue that the steady-state current $I_L$ in an extended quantum system connected to two leads $L$ and $R$ evaluated according to [2–7]

$$I_L = I_{LB} = \frac{2e}{h} \int_{-\infty}^{\infty} d\epsilon \text{tr} \{ (f_L - f_R) \left( \Gamma_L G^+ \Gamma_R G^- \right) \}$$ (1)

is not consistent with $I$ when calculated with the other established formula [6–8]

$$I_L = I_{MW} = \frac{ie}{h} \int_{-\infty}^{\infty} d\epsilon \text{tr} \left[ (f_L \Gamma_L - f_R \Gamma_R) (G^+ - G^-) + (\Gamma_L - \Gamma_R) G^- \right]$$ (2)

(for finite systems they claim $I_{LB} = I_{MW}$). We use the standard notations where $f_\alpha \equiv f_\alpha(\epsilon - \mu_\alpha)$ is the distribution function on the left ($\alpha = L$) or right ($\alpha = R$) lead with the chemical potential $\mu_L$ ($\mu_R$) and $\Gamma_\alpha = i(\Sigma^-_\alpha - \Sigma^+_\alpha)$, where $\Sigma^\pm_\alpha$ is the respective selfenergy. The superscript $(--)$ stands for retarded (advanced) quantities. The operators $G^\pm$ satisfy a Dyson equation that can be written as

$$G^\pm = \left[ g^\pm_c - (\Sigma^\pm_L + \Sigma^\pm_R) \right]^{-1}$$ (3)

hereby $g_c(z) = (z - H_c)^{-1}$ is the resolvent of $H_c$, which is a hermitian Hamiltonian describing the isolated central region and $g^\pm_c(z) = g_c(\epsilon \pm i\eta)$ where $\eta$ is a small positive real number taken to zero after performing the trace and the energy integration in eq.(1,2). $G^- = iG^+ (f_L \Gamma_L + f_R \Gamma_R) G^-$ (cf. 7).

Zhou and Wu claim that our previous results [9, 10] calculated with eq.(1), and for that matter the results of all other researchers employing the same approach for an extended system, lack scientific ground. Let us show mathematically that the inconsistencies found by Zhou and Wu when using eq.(1) vs. eq.(2) are self-made and indeed eq.(1) and eq.(2) should yield consistent results independent of whether the system is finite or extended (in the sense introduced by Zhou and Wu in Ref.[1]).

For clarity let us work in a representation free manner and write the operator equation

$$(G^+ - G^-) = G^+ \left( G^{-1} - G^{+1} \right) G^-$$

which readily yields (cf. eq.[3])

$$G^+ - G^- = G^+ \left[ (\epsilon - i\eta - H_c) - (\epsilon + i\eta - H_c) \right] G^- - iG^+ (\Gamma_L + \Gamma_R) G^-$$ (4)

$$= -2i\eta G^+ G^- - iG^+ (\Gamma_L + \Gamma_R) G^-.$$ (5)

The trace of this equation is to be compared with the eq.(5) in Ref.[1]. Zhou and Wu claimed that the first term in Eq. (4) vanishes ... in the finite system, in consistence with the previous literature. However, in the infinite system discussed by Ding et al. [2] the situation...
becomes totally different. Hence, they derive a "new correct formula" for extended systems by taking the first term of Eq. (5) into account and construct a way to make it finite.

As a matter of fact for a finite $\Gamma_\alpha$, mathematically the trace of the first term of Eq. (5)

$$-2i\eta G^+ G^- = G^+ [(\epsilon - i\eta - H_c) - (\epsilon + i\eta - H_c)] G^-$$

(6)

has to vanish always and in any basis when $\eta \to 0$, for in this case $G^\pm$ has neither isolated poles nor a branch cut for $\eta \to 0$, i.e. when approaching the real energy axis. This is also evident from the structure of $G^\pm$ (cf. 3). For $\Gamma_\alpha \to 0$, the trace over $-2i\eta G^+ G^-$ yields for $\eta \to 0$ indeed the spectral density of the system, and the second term of Eq. (5) is identically zero. This is consistent with the well-established meaning of the trace over $G^+ - G^-$. For $\Gamma_\alpha \to 0$ however the current $I_{MW}$ vanishes as clear from eq.(2). This means in turn that introducing somehow a finite trace over $-2i\eta G^+ G^-$ for $\eta \to 0$ regardless of $\Gamma_\alpha$ being finite, amounts to a change of the system spectral density and raises thus the question of the charge conservation (i.e. $I_R = -I_L$). Indeed, as well-established and readily deducible from both prescriptions (1) and (2) the charge conservation is fulfilled for (1) and (2). Constructing somehow a finite trace of the term (6) one may enforce as an additional condition that $I_R + I_L = 0$ and distribute accordingly the spurious term on $I_L$ and $I_R$, such an approach to restore the charge conservation, however, is far from being fundamental!

We infer mathematically thus that for steady-state transport, i.e. when $\Gamma_\alpha$ is finite, the first term of Eq. (4) plays no role.

Nonetheless, Zhou and Wu argue that the term $-2i\eta G^+ G^-$ should be finite because in eq.(4) one may write (cf. eq.(5) in Zhou and Wu comment)

$$G^+ [(\epsilon - i\eta - H_c) - (\epsilon + i\eta - H_c)] G^- = G^+ [g_c^{-1} - g_c^{+1}] G^-$$

(7)

and assume a finite $(g_c^{-1} - g_c^{+1})$. While one may do such a manipulation the contribution of this term to the current remains of course zero [11]. Clearly, replacing a vanishing term by an energy and momentum dependent function may lead to a series of conclusions that are at variance with known results, including the statement that eq.(1) is not applicable for an extended system.

The matter of fact however, for a finite $\Gamma_\alpha$ only the second term of eq.(5) contributes when taking the trace in eqs.(12) and letting $\eta \to 0$. It is straightforward to show by
inserting eq.(5) into eq.(2) that one retrieves the established result

\[ I_L = \frac{e}{\hbar} \int_{-\infty}^{\infty} d\epsilon \text{tr} \left\{ (f_L - f_R) \left[ \begin{array}{cc} \Gamma_L G^+ \Gamma^- \Gamma_R G^+ & \Gamma_R G^+ \Gamma_L G^- \end{array} \right] \right\} \] (8)

which is equivalent to eq.(1) that we and others use for the calculation of the steady-state current.

Hence, as far as the system size is concerned, as introduced by Zhou and Wu and we only focus on this issue here, one may use eq.(1) or eq.(2) and finds \( I_{LB} = I_{MW} \). More importantly any effects on the transport based on a finite first term in eq.(5) should be considered artificial and resulting from some uncontrolled approximations. Based on their "correct" formula Zhou and Wu go even a step further in their conclusions and state that works for an extended system employing eq.(1) are incorrect and lack scientific ground. This statement is clearly a consequence of a self-made finite term that for a finite current should be in fact zero due to fundamental reasons.

Based on their new, allegedly "correct" formula Zhou and Wu raise some issues concerning our results [9, 10], in particular those for the tunnel magnetoresistance (TMR) of a graphene monolayer contacted to metallic ferromagnetic leads that we obtained on the basis of eq.(1). Since our results do not agree with their calculations based on their own constructed formula they claim that the reason is due to a "wrong" energy cutoff \( D \) that we use in our calculation. It should be noted, that as shown by Zhou and Wu the spurious term they include in their formula contains \( D \) in a non-trivial manner. In their comment [1] they make several claims based on the dependence of their calculated current on \( D \). While this point is somehow technical, a clarification might be useful to avoid a misunderstanding of the meaning of \( D \).

We choose \( D \) as to ensure the conservation of the number of states in the Brillouin zone (upon linearizing the spectrum, cf. Ref.[12]). Calculating \( D \) accordingly one arrives at the Green function given in our works. This is a physically motivated way to choose \( D \) that can be set as the energy scale. Of course, one may choose another \( D \) which in turn means a violation of the number of states in the Brillouin zone.

As shown in Figs.1,2, we can perform the calculations using \( D \) or \( \Gamma_0 \) (\( \Gamma_\alpha \) are assumed to be momentum and energy independent) as the energy scale and arrives at the same behaviour of the TMR. Proceeding as suggested in the comment by Y. Zhou and M.W. Wu one arrives at an opposite physical behaviour of TMR, i.e. a zero TMR at zero bias instead of a peak. Indeed, it is straightforward to show analytically, that this behaviour is a direct consequence
FIG. 1. (color online) TMR in a graphene monolayer in contact with two metallic ferromagnetic leads as a function of the applied bias $V$, calculated according to eq.(1) or eq.(2) while correctly neglecting the first term of eq.(5) (as done in our previous work [9]). The dots are the results derived by setting the energy width $D$ as the unit of energy. The solid line is the result by using the broadening function $\Gamma_0$ as the unit of energy. $D/\Gamma_0 = 12$ and the spin polarization of the two metallic ferromagnetic leads is 40%. The leads are assumed to be of the same material.

of assuming, as done by Zhou and Wu, a finite first term in eq.(2) that is related to the spectral density of graphene. In addition, in their comment Zhou and Wu show the result of their "correct" formula for the conductance. It can be shown mathematically that the behaviour of the conductance at small bias in their case is dominated by the erroneous finite first term in eq.(5).

In Summary, eq.(1) and eq.(2) are valid irrespective of whether the system is finite or extended (in the sense mentioned in the comment). The claims of Y. Zhou and M.W. Wu in their comment are the result of a fabricated finite energy and momentum-dependent term that should vanish due to fundamental reasons if the current is finite. Established approaches to quantum transport are consistent within the well-documented limits.
FIG. 2. (color online) as in Fig. 1, however the TMR is calculated by using the suggestion by Zhou and Wu in Ref. [1]. The parameters are the same as those in Fig. 1. Note, we do not consider Eq. (18) of Zhou and Wu in our numerics. We stress that, as stated in the figure caption, our Fig. 2 is obtained as Fig. 1 from our theory, but we include in the calculations a constructed finite spurious term of the form given by Eq. (7), along the line as we understand the suggestion by Zhou and Wu. Note, as discussed above, in this case the charge conservation is not a priori guaranteed.

[1] Y. Zhou and M. W. Wu, preceding comment.
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[11] This is also obvious when working with the momentum \( q \) states of graphene, in which case the graphene Green’s is diagonal and reads

\[
g_{q,q}(\varepsilon) = \frac{1}{\varepsilon \pm i\eta - q_x\sigma_x - q_y\sigma_y}
\]

(9)

and the Green function for the composite structure satisfies the Dyson equation

\[
G_{q,q'}(\varepsilon) = \delta_{qq'}g_{q,q}(\varepsilon) + \sum_{q_1} g_{q,q}(\varepsilon)\sigma^+\Sigma_{q_1}^+(\varepsilon)G_{q_1,q'}(\varepsilon)
\]

(10)

where \( \sigma^+ = \frac{1}{2}(1 + \sigma_z) \). With these expressions, it is readily inferred that taking the trace in (7) and letting \( \eta \rightarrow 0 \) the term given by eq. (7) vanishes.

[12] B. Uchoa, V. N. Kotov, N. M. R. Peres, and A. H. Castro Neto, Phys. Rev. Lett. 101, 026805 (2008).