

Green's function  $\hat{\mathbf{G}}$  of the embedded molecule as

$$\hat{\mathbf{G}}^{-1} \simeq \hat{\mathbf{G}}_{i,0}^{-1} - \hat{\Sigma}_{i,corr} - \hat{\Sigma}_{0,L} - \hat{\Sigma}_{0,R} , \quad (13)$$

$$\hat{\mathbf{G}}^{-1} \simeq \hat{\mathbf{G}}_i^{-1} - \hat{\Sigma}_{0,L} - \hat{\Sigma}_{0,R} , \quad (14)$$

provided that one is able to accurately compute the matrix Green's function  $\hat{\mathbf{G}}_i$  of an isolated, but still sufficiently large extended molecule. In view of the physical motivation behind it, we shall refer to the approximation involved in Eqs. (13) and (14) as the approximation of a sufficiently large extended molecule. This concept plays a central role for all the subsequent considerations of the present paper.

According to Eq. (14), to compute the full matrix Green's function  $\hat{\mathbf{G}}$  of a sufficiently large extended molecule, in addition to  $\hat{\mathbf{G}}_i$ , one only needs  $\mathbf{\Gamma}_x$  and  $\hat{\Sigma}_{0,x}$  ( $x = L, R$ ). More precisely, what one only needs is the retarded self-energy  $\Sigma_{0,x}^r$ , because all the other quantities can be expressed in terms of it as follows [16, 25]

$$\begin{aligned} \mathbf{\Gamma}_x &= i \left[ \Sigma_{0,x}^r - (\Sigma_{0,x}^r)^\dagger \right] , \\ \Sigma_{0,x}^< &= i f_x \mathbf{\Gamma}_x , \\ \Sigma_{0,x}^> &= -i (1 - f_x) \mathbf{\Gamma}_x . \end{aligned} \quad (15)$$

Consequently, the hard part to calculate the current is to obtain the matrix Green's function  $\hat{\mathbf{G}}_i$  of the isolated extended molecule. [As shown below, it even suffices to compute the retarded block  $\mathbf{G}_i^r$ , cf. Eqs. (17) and (16).] By inserting Eqs. (3), (5), (6), and (15) into Eq. (1), one can express the steady-state current through a sufficiently large extended molecule as

$$I \simeq \frac{e}{h} \int d\varepsilon \text{Tr} [f_L(\varepsilon) - f_R(\varepsilon)] \mathbf{\Gamma}_L(\varepsilon) \mathbf{G}^r(\varepsilon) \mathbf{\Gamma}_R(\varepsilon) \mathbf{G}^a(\varepsilon) . \quad (16)$$

In the absence of correlations  $\mathbf{G}^{r,a} \rightarrow \mathbf{G}_0^{r,a}$ , Eq. (16), which reduces to the familiar Landauer formula, is an exact result probably first deduced in Ref. 26 and often discussed later, e. g. [16, 18, 25, 27, 28]. Although similar to the uncorrelated case, Eq. (16) does account for electron correlations, because  $(\mathbf{G}^{r,a})^{-1} - (\mathbf{G}_0^{r,a})^{-1} \simeq -\Sigma_{i,corr} \neq \mathbf{0}$ . It becomes similar to Eq. (10) of Ref. 16, deduced for proportionate coupling, if one approximates  $\Sigma \simeq \Sigma_0$  there, in the spirit of the present paper. It is also similar to Eq. (17) of Ref. 25; if the correction factor used there is set to unity ( $\Lambda = 1$ ), that equation coincides with the present Eq. (16). The physical motivation of the coincidence of these two equations is clear: as seen