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GW approach to electron-electron interactions within the Anderson impurity model: Kondo correlated quantum transport through two coupled molecules

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A B S T R A C T

We invoke the nonequilibrium self-consistent GW method within the Anderson impurity model to investigate the dynamical effects occurring in a nanojunction comprised of two coupled molecules. Contrary to the previous single impurity model calculations based on the GW approximation, we observe that the density of states manages to capture both the Kondo resonance and the Breit-Wigner resonances associated with the HOMO and LUMO levels of the molecule. Moreover, the prominence of the Kondo resonance grows dramatically upon switching from the intermediate to the weak coupling regime involving large U/Γ values. The conductance is calculated as a function of the HOMO level and the applied bias across the molecular nanojunction. Calculated conductance curves deviate from the monotonic decay behaviour as a function of the bias when the half-filling condition is not met. The importance of the effect of the molecule-molecule coupling for the electron transport phenomena is also investigated.

Nonequilibrium Green function theory provides a systematic framework to overcome some of the shortcomings that arise while treating the strong electron correlations within the Kohn-Sham based density functional theory (DFT), which accounts for the electron-electron interactions only in the mean field level. Although the DFT based NEGF theories have been successfully applied for the electron transport when the coupling between the impurity and the bath is strong [1,2], they turn out to be insufficient for the weak coupling regime where the electron-electron correlation effects dominate. A suitable choice to approximate the electron self-energy that is expected to represent the electron-electron correlations properly remains crucial. In order to obtain an accurate description of electron transport within NEGF approach, one needs to utilize conserving approximations. One of the most widely used and conserving approximations to the self-energy is the many-body GW approximation [3], where W stands for the dynamically screened interaction. The GW self-energy must be obtained via the functional derivative of Φ[G] of the Green function to satisfy the conservation laws and then solved fully self consistently within the framework of Dyson equations [4–6].

Due to the computational cost of GW, one can resort to the restricted scheme of GW or semi conserving methods like GW_0 and G_0W_0 in most applications. This choice may not matter for the investigation of the spectral properties but is critical for the out-of-equilibrium quantum transport [4,7]. Although G_0W_0 approximation shows compatible results with experiment it is not a conserving approximation in the Kadanoff-Baym sense [8] and leads to the non-conservation of the number of particles. Another important issue is how to construct interactions and incorporate them into the calculations involving GW approximation where the electron-electron correlations are encoded via the choice of a self-energy operator.

In general, GW does not provide an entirely correct description of the spin correlations between the impurity and lead electrons. There are methods [9], which provide a remedy for this inadequacy by taking into account the spin dependent interactions based on the generalized Hedin equations and $\sigma G\sigma W$ approximation [10]. Within $\sigma G\sigma W$ approximation it is possible to obtain universal scaling behaviour in the Kondo regime but it is not fully satisfactory.

The GW approximation has been used for the single impurity Anderson model without accounting for the spin-flip processes properly [4,9]. Nevertheless, this approach still managed to capture the Kondo resonance within certain parameters in Kondo regime. In addition, results from these studies also indicate that this method fails to capture, especially for large U/Γ, Breit-Wigner resonances at the atomic levels HOMO and LUMO [4]. On the other hand, the low energy properties of the single impurity Anderson model with spin-flip processes built in yield far more superior results compared to the nonspin-flip case [9]. GW approximation also shows distinctly different behaviour with respect to the coupling strength between the leads and the atomic levels.

Exploring the Kondo physics also requires applying a voltage bias such that it is sufficiently small compared with the Kondo temperature [11,12]. Moreover, the nonequilibrium GW studies present hysteresis in I-V characteristics at some applied bias [13] which means there is more than one steady state solution. Within the GW approximation,

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when the ambient temperature lies below the Kondo temperature, the spectral properties don't appear to be reliable in the case of zero-bias [11]. When the applied bias is increased the differential conductance starts to dwindle. In large bias, Kondo peak splits and the width of individual peaks gets broadened [4,11]. According to a previous work [6], the Kondo peak does not appear in the regime of intermediate coupling since the GW approximation leads to broken spin symmetry. On the other hand it has been shown that GW approximation for weak electron-electron interactions reflects the impact of spin in the single impurity Anderson model [6] remarkably well.

Obtaining accurate results in the weak coupling regime has so far been quite elusive within the GW approximation and it is our aim in this letter to tackle this issue. Towards this end, we will use a junction consisting of two coupled molecules. We will investigate the behaviour of the density of states and the conductance of this system systematically. We will show for the first time that the GW approximation can indeed provide reliable results even for strong interaction strengths where U/Γ value exceeds 8.

We theoretically model this system with a three piece Hamiltonian $H = H_L + H_s + H_R$ where L, R and s denote the left, right leads and the central region respectively. The leads are kept at chemical potentials μ_L and μ_R. The central region consists of two coupled molecules and its Hamiltonian is given by $H_s = H_{m_1} + H_{m_2} + H_{m_1m_2}$ in which m_1 and m_2 denote the first and second molecule. We depict the system under consideration schematically in Fig. 1. The total Hamiltonian in the second quantized form for this system turns out to be

$$H = \sum_{K,\sigma} \varepsilon_K c^{\dagger}_{K\sigma} c_{K\sigma} + \sum_{s,\sigma} \varepsilon_s c^{\dagger}_{sg\sigma} c_{sg\sigma} + \sum_{s,\sigma} (\varepsilon_s + U) c^{\dagger}_{se\sigma} c_{se\sigma} + \sum_{K,s,\alpha,\sigma} (t_{K,s} c^{\dagger}_{K\sigma} c_{s\alpha\sigma} + h.\,c.\,) + \sum_{m_1,m_2,\alpha,\sigma} (t_{m_1m_2} c^{\dagger}_{m_1\alpha\sigma} c_{m_2\alpha\sigma} + h.\,c.\,) + \frac{U}{2} \sum_{s,\alpha,\sigma} n_{s\alpha\sigma} n_{s\alpha\sigma'}, \quad (1)$$

where K denotes the left L and right R electrodes and s stands for each molecule ($s \in \{m_1, m_2\}$) which consists of two discrete levels called HOMO and LUMO. These levels are denoted with $|g\rangle$ and $|e\rangle$. Moreover, ε_s and $\varepsilon_s + U$ correspond to the energies of the HOMO and LUMO level in each molecule respectively. Thus, the charging energy U amounts to the HOMO-LUMO energy gap as it should. $c^{\dagger}_{K\sigma}(c_{K\sigma})$ and $c^{\dagger}_{sg(e)\sigma}(c_{sg(e)\sigma})$ create (annihilate) an electron in the metal electrodes and in each discrete atomic level within the molecules respectively. U and $n_{sg(e)\sigma}$ denote the Coulomb interaction and the number operator. We represent the molecule-lead coupling parameter shortly as $t_h = t_{K,s}$ and molecule-molecule hopping as $t_m = t_{m_1,m_2}$.

We consider a simple case of two identical leads, i.e chemical potentials are given by $\mu_{L/R} = E_F \pm \frac{V}{2}$ where V is the applied bias voltage and E_F is the Fermi level and in this study we set the $E_F = 0$. We also assume that there is no direct coupling between two leads. We follow the nonequilibrium GW approach [4,7] to investigate the electronic properties and quantum transport phenomena within tight-binding model.

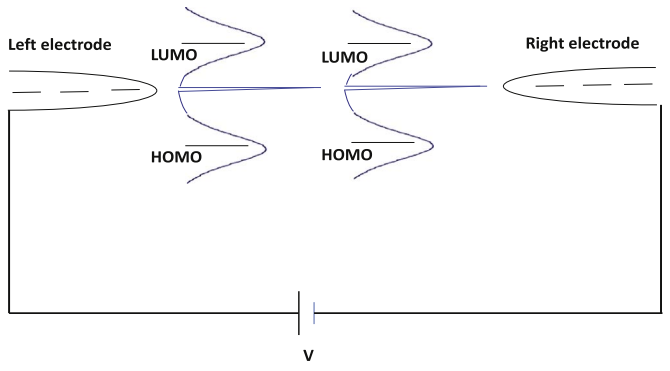

Fig. 1. This figure illustrates the one dimensional tight binding model where we insert two coupled HOMO-LUMO energy levels which mimic the two connected molecules.

Lesser and greater GW self energies are given as follows [6]

$$\Sigma^{<}_{ij}(t) = iG^{<}_{ij}(t) W^{<}_{ij}(t), \quad (2)$$

$$\Sigma^{>}_{ij}(t) = iG^{>}_{ij}(t) W^{>}_{ij}(t). \quad (3)$$

Based on these expressions, the well known retarded GW self-energy can be written as

$$\Sigma^{r}_{ij}(t) = -i\Theta(t)(\Sigma^{>}_{ij}(t) + \Sigma^{<}_{ij}(t)) = -i\Theta(t)(iG^{>}_{ij}(t) W^{>}_{ij}(t) + iG^{<}_{ij}(t) W^{<}_{ij}(t)) \quad (4)$$

Here t denotes the time difference $t' - t$. After applying Langreth rules [14] one can finally reach the retarded self energy in terms of the retarded Green function and the retarded screened function

$$\Sigma^{r}_{ij}(t) = iG^{r}_{ij}(t) W^{>}_{ij}(t) + iG^{<}_{ij}(t) W^{r}_{ij}(t) \quad (5)$$

where $W^{r}_{ij}(t)$ is defined as

$$W^{r}_{ij}(t) = -i\Theta(t)(W^{>}_{ij}(t) - W^{<}_{ij}(t)) \quad (6)$$

We can also write retarded, lesser and greater screened interactions in frequency space as

$$W^{r}(w) = \widetilde{V}[I - P^{r}(w)\widetilde{V}]^{-1} \quad (7)$$

and

$$W^{<\,/\,>}(w) = W^{r}(w) P^{<\,/\,>}(w) W^{a}(w) \quad (8)$$

On the other hand, irreducible polarization terms are given by

$$P^{r}_{ij}(t) = -iG^{r}_{ij}(t) G^{<}_{ij}(-t) - iG^{<}_{ij}(t) G^{a}_{ij}(-t)) \quad (9)$$

$$P^{<\,/\,>}_{ij}(t) = -iG^{<\,/\,>}_{ij}(t) G^{>\,/\,<}_{ji}(-t) \quad (10)$$

In all calculations, the effective interaction [4,7] $\widehat{V_{eff}} = \frac{1}{2}\Sigma_{ij} \widetilde{V}_{ij} c^{\dagger}_i c^{\dagger}_j c_i c_j$ where $\widetilde{V}_{ij} = V_{ij,ij} - \delta_{\sigma\sigma'} V_{ij,ji}$ is used. It is understood that $\widetilde{V}_{ij}$ is spin dependent and self interaction is excluded [4].

All HF and GW calculations were performed using the GPAW [15] code where the current formula [16] is implemented through

$$I_\alpha = \int \frac{d\omega}{2\pi} Tr[\Sigma^{<}_{\alpha}(\omega) G^{>}_{C}(\omega) - \Sigma^{>}_{\alpha}(\omega) G^{<}_{C}(\omega)] \quad (11)$$

Here α denotes the L or R leads respectively and the net steady state current can be obtained by using $I = (I_L - I_R/2)$.

The GPAW is a nonequilibrium Green function (NEGF) based density functional theory (DFT) code that allows investigation of the optical and electronic properties by taking into account both the electronic correlations and exchange effects. The advantage of using a DFT based methodology is to obtain self consistent results after setting up the initial Green functions that describe the non-interacting leads and a scattering Hamiltonian. Calculations are called for the self consistent GW after obtaining the initial non-interacting Green function. The main reason why we use the tight binding model is its simplicity. Besides, the model gives good qualitative results that mimic the reality fairly well. We refer to the GPAW web page for further details and other references that invoke it.

In our calculations, we tune the interaction strength U/Γ from 2 to 20 while keeping U=4.0. We set the Fermi level at $E_F = 0$ and the frequency grid extends from −10 to 10.

In Fig. 2, we show the equilibrium spectral function for HF and GW solutions corresponding to various values of the atomic level ε_s. The calculation is performed using U=4.0, molecule-molecule hopping $t_m = 1.5$ and molecule-lead coupling $\Gamma = 0.20$ corresponding to $U/\Gamma = 20$. For $\varepsilon_s = -3.0$ both HF and GW Kondo peaks are pinned to the Fermi level. However, when ε_s deviates from this value, the position of the Kondo peak starts to shift to the right or left. The full width at half maximum (FWHM) of the Kondo peak is given approxi-

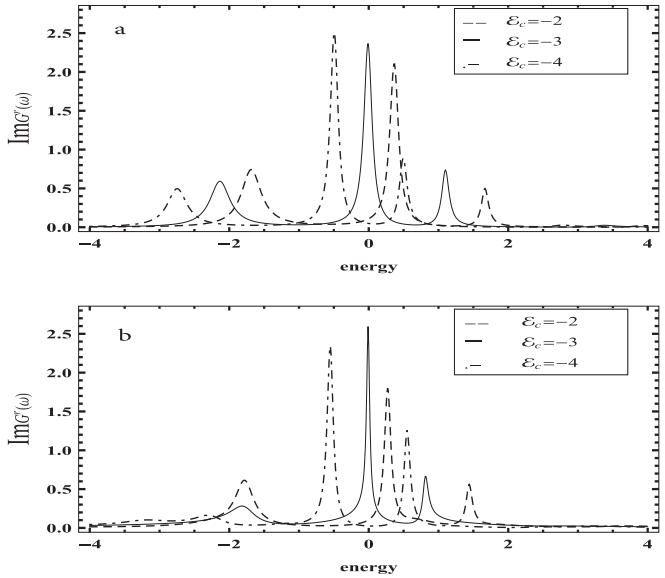

Fig. 2. This figure illustrates spectral properties for different HOMO values for HF (panel a) and GW (panel b) method. We use $\varepsilon_s = -2.0$, $\varepsilon_s = -3.0$, $\varepsilon_s = -4.0$ HOMO energy values with U=4.0, t_m = 1.5 and Γ = 0.20.

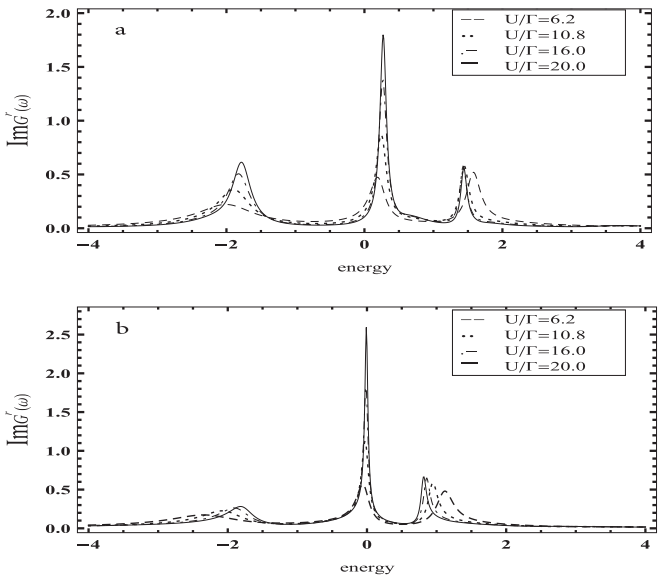

Fig. 4. This figure illustrates spectral function of GW method for the central cite with different U/Γ values. Here, for panel a $\varepsilon_s = -2.0$ and for panel b $\varepsilon_s = -3.0$ is used. For both panels t_m = 0.4 and U=4.0 values are chosen.

mately by the Kondo temperature [17]

$$T_K \approx 0.5\sqrt{2\Gamma U}\,\exp[\pi\varepsilon_s(\varepsilon_s + U)/2\Gamma U]. \quad (12)$$

FWHM of our GW Kondo peaks satisfies this exponential scaling of T_K quite well in agreement with the previous work [4] as one can clearly see in Fig. 3. We observe this exponential scaling for all ε_s values upon sweeping U/Γ. Nevertheless, numerical results start to differ from analytical predictions slightly when U/Γ is lowered because the Kondo resonance starts to get quenched in this regime. It is important to point out that we manage to retain exponential scaling at elevated U/Γ values in contrast with the previous work [9], which yields algebraic scaling. This error stems from incorrect spin correlations between the molecule and the lead electrons in the single impurity problem [9]. We restore these correlations by turning on the molecule-molecule coupling for the first time. Deviations from this exponential scaling increase considerably for the HF calculations as one can easily notice the relative broadening of Kondo resonances in Fig. 2. This is not surprising since HF approximation is well known to be cruder than GW approximation to account for strong electron correlations.

On the other hand, the FWHM of the Breit-Wigner resonance associated with the HOMO level scales with Γ for both the HF and GW

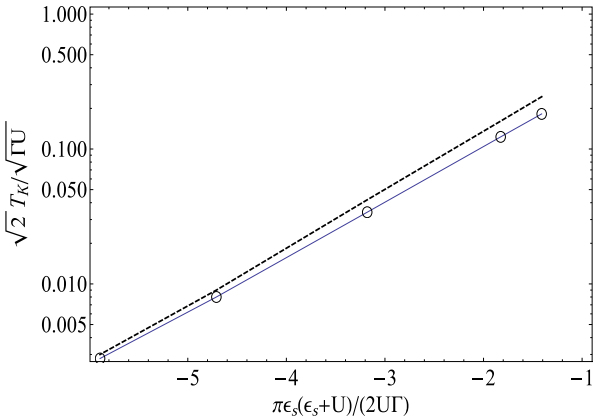

Fig. 3. This figure shows comparison of the FWHM of the Kondo peak obtained from numerical calculations involving GPAW for various values of U/Γ and ε_s=−3 with the analytical result given by Eq. (12). Empty circles denote the numerical results whereas dashed curve represents the analytical result.

solutions since it originates from the lifetime broadening arising due to the hybridization of the leads with the molecule. Furthermore, the position of the Breit-Wigner resonance associated with the HOMO level tends to move away from ε_s when ε_s starts to shift downwards from the Fermi level for GW calculations. This is certainly unrealistic and it needs to be checked whether this pathological situation remains robust upon tuning U/Γ.

Towards this end, we investigate the dependence of the spectral function on the ratio U/Γ for $\varepsilon_s = -2.0$ and $\varepsilon_s = -3.0$ in Fig. 4. We use $\varepsilon_s = -2.0$ for panel a, $\varepsilon_s = -3.0$ for panel b and set t_m = 0.4, U=4.0 for both panels. We see that the sharpness of the Kondo peak grows dramatically when U is much larger than the molecule-lead hybridization energy, Γ. These results are in stark contrast with previous GW studies which failed to demonstrate the existence of the Kondo peak in the regime where $U/\Gamma > 8$ [4,6]. These earlier works involve a single molecule coupled to the continuum which is modeled by the wide-band approximation. This naturally results in a smeared out Kondo resonance for strong interaction strengths. We overcome this deficiency in this paper by using two molecules which are coupled to each other and the continuum simultaneously. Turning on the molecule-molecule coupling in this manner enables to restore the spin symmetry and thus the survival of the Kondo resonance is ensured. Therefore, our results represent a major breakthrough for the exploration of strong electron correlations via the GW method.

In Fig. 4, the position of the Kondo peak for $\varepsilon_s = -3.0$ remains pinned to the Fermi level upon increasing U/Γ, whereas it gets shifted to the right slightly for $\varepsilon_s = -2.0$. On the other hand, reducing U/Γ to around 15 largely restores the position of the Breit-Wigner resonance associated with the HOMO level for $\varepsilon_s = -2.0$. As for $\varepsilon_s = -3.0$, the Breit-Wigner resonance associated with the HOMO level is still away from ε_s even when U/Γ falls well below 10. It is also important to note that reducing U/Γ quenches both the Kondo resonance and the Breit-Wigner resonances associated with the HOMO and LUMO levels. Therefore, it is detrimental to stick with U/Γ values smaller than 10 if one wants to describe the dynamics of this system accurately.

Further investigation of the spectral function for $\varepsilon_s = -3.0$ is displayed in Fig. 5. We keep reducing U/Γ value here such that the Kondo resonance starts to diminish to the point of extinction. It is clear from this figure that the Breit-Wigner resonance on the left hand-side of the Fermi level is still not centered around ε_s even at very low U/Γ values. In this regime, the Breit-Wigner resonance associated with

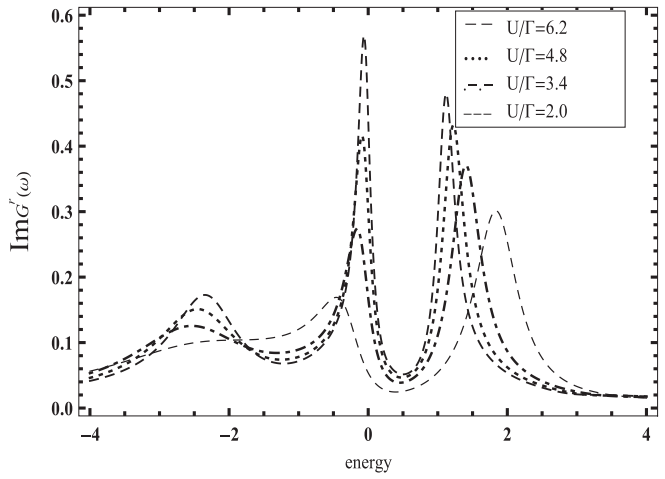

Fig. 5. This figure illustrates the spectrum for GW method using large Γ values with U=4.0 and $\varepsilon_s = -3.0$, $t_m = 0.4$.

LUMO level on the right hand-side of the Fermi level starts to shift away from $\varepsilon_s + U$ position as well. Therefore, it is reasonable to conclude that the GW approach fails to locate the resonances properly and sharply enough if the HOMO level starts to move away from the Fermi level.

We now want to study the implications of the spectral properties on the electron transport through this system. In Fig. 6, we show the zero-temperature conductance under a symmetric bias, $\mu_{L/R} = \pm\frac{V}{2}$, as a function of bias for $\varepsilon_s = -2.0, -3.0, -4.0$ HOMO levels and we use the parameters U=4.0, $t_m = 1.0$ and $\Gamma = 0.20$. Apart from a tiny deviation near zero bias, the conductance curve for $\varepsilon_s = -2.0$ exhibits smooth decay behaviour until large bias values as expected. The underlying mechanism for this behaviour is the splitting of the Kondo peak into two at finite bias. As the bias is ramped up, split Kondo peaks start to dwindle and disappear eventually at large bias. This gives rise to a monotonic suppression of the conductance. However, this situation changes when the HOMO level starts to move away from the Fermi level. In Fig. 6, conductance curve for $\varepsilon_s = -3.0$ develops a small plateau when the bias reaches around 3 resulting in a slight deviation from the monotonic decay behaviour. This plateau becomes even more prominent for the conductance curve corresponding to $\varepsilon_s = -4.0$. This causes an unrealistic increase in the conductance around the bias value of 2 ruining the smooth decay behaviour completely.

We attribute the gradual deterioration of the conductance curves as

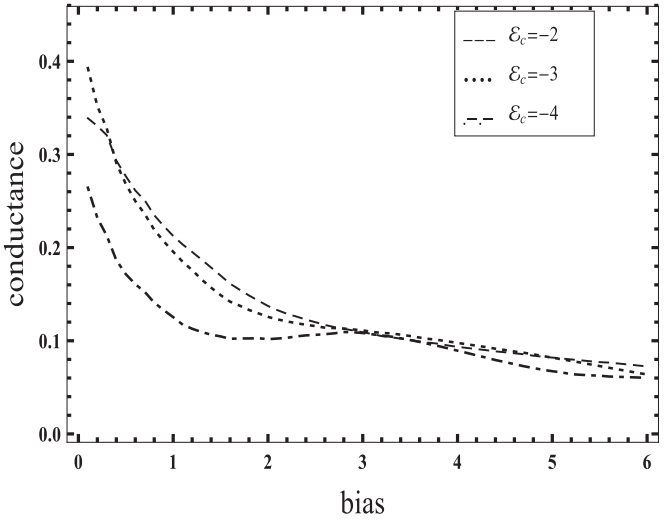

Fig. 6. Conductance as a function of bias for GW method with $t_m = 1.0$, $\varepsilon_s = -2.0, -3.0, -4.0$, $\Gamma = 0.20$ and U=4.0.

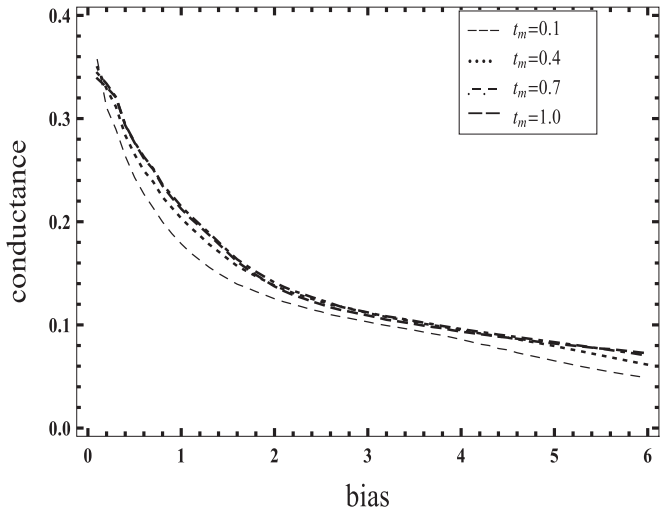

Fig. 7. Conductance as a function of bias and different molecule-molecule coupling for GW method, t_m with $\varepsilon_s = -2.0$, $\Gamma = 0.20$ and U=4.0.

ε_s shifts away from the Fermi level to the incorrect positioning of the resonances in the spectral function. The Kondo resonance is supposed to be located slightly above the Fermi level while the Breit-Wigner resonances associated with HOMO and LUMO levels should be located around ε_s and $\varepsilon_s + U$ [18]. The spectral function for $\varepsilon_s = -2$ reflects this most accurately therefore its conductance curve exhibits the smooth decay behaviour. We think the emergence of a plateau in the conductance curve for $\varepsilon_s = -3$ and $\varepsilon_s = -4$ is related to the misalignment of the resonances in their spectral functions.

In Fig. 7, we investigate how the conductance changes upon varying the molecule-molecule hopping parameter, t_m. We stick with $\varepsilon_s = -2$ in this case since this value of the HOMO level describes the behaviour of the conductance as a function of the bias most accurately as we have seen in Fig. 5. This can be ascribed to the fact that the Kondo temperature takes its minimum value when half-filling occurs, i.e. $\varepsilon_s = -U/2$. This type of behaviour is observed whenever $\varepsilon_s + U/2 = 0$ condition is satisfied. [6]. Consequently, the value of Coulomb interaction strength U is of critical importance and calculations involving ε_s parameters that don't satisfy the above criterion generate unrealistic results.

When t_m is taken to be zero, the conductance vanishes for all bias values since the circuit is open in this configuration. As soon as the hopping is turned on, we observe a sudden jump in the conductance in Fig. 7 because the electron transport is enabled. The conductance starts to increase slightly for all bias values when the hopping is ramped up saturating eventually at large values of t_m. This is simply because the electron tunneling rate is so fast anymore such that boosting t_m any further makes equal contribution to the left and right currents. It is also worth emphasizing that the smooth decay behaviour is maintained for all values of t_m.

In this letter, we demonstrated for the first time invoking GW method that the density of states of a nanojunction made up of two coupled molecules exhibits both the Kondo resonance and the Breit-Wigner resonances associated with the HOMO and LUMO levels of the molecule. We showed that the correct positioning of these resonances requires a careful calibration of the HOMO level of the molecule and the accurate alignment of the resonances occurs only when the half-filling condition is met, namely when the HOMO level is positioned at half the value of the Hubbard interaction strength below the Fermi level. Moreover, we compute the density of states of two coupled impurities via GW method for the first time and show that not only the Kondo resonance survives when the Hubbard interaction strength overwhelms the molecule-lead coupling but its prominence grows dramatically contrary to the previous studies [4,6]. We also studied

the conductance of such a device and our results indicate that the conductance is suppressed monotonically as a function of the applied bias for all molecule-molecule couplings if the half-filling condition is satisfied. Unrealistic plateaus start to appear in the conductance at finite bias values away from the half-filling ruining the monotonic decay behaviour.

Our results clearly represent a pioneering achievement towards investigating strongly correlated nano junctions via the GW method and will certainly pave the way for accurate theoretical predictions for complex systems in the future. This will hopefully motivate and spur further experiments in this rapidly evolving field.

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