Spin current through an ESR quantum dot: A real time study

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The spin transport in a strongly interacting spin-pump nano-device is studied using the time-dependent variational-matrix-product-state (VMPS) approach. The precession magnetic field generates a dissipationless spin current through the quantum dot. We compute the real time spin current away from the equilibrium condition. Both transient and stationary states are reached in the simulation. The essentially exact results are compared with those from the Hartree-Fock approximation (HFA). It is found that correlation effect on the physical quantities at quasi-steady state are captured well by the HFA for small interaction strength. However the HFA misses many features in the real time dynamics. Results reported here may shed light on the understanding of the ultra-fast processes as well as the interplay of the non-equilibrium and strongly correlated effect in the transport properties.

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I. INTRODUCTION

The rapid progress of nano-electronics and information technologies has prompted intense interest in exploiting the spin properties of the electrons, which results in the emergence of spintronics.¹ One of the most important spin-based electronic devices is a mesoscopic quantum dot (QD) system. Spin-polarized transport through a QD has been extensively investigated recently. It has been shown theoretically ² and demonstrated experimentally ³ that a QD system will function as a phase-coherent spin pump in the presence of sizable Zeeman splitting. Very recently, spin-polarized current has been detected from a quantum point contact (QPC) ⁴ and from Coulomb-blocked QDs ⁵. The electron spin resonance QD (ESR-QD) could also serve as an element device for quantum computing.⁶

Due to its small size, Coulomb correlation could play important role in the transport experiments involving a QD. At low temperature, Kondo effect creates new states with many-body character at the Fermi level. Although the effect of Kondo resonance on the charge current has been studied in the QD for different situations, its influence on the spin current is less known. The physical processes involved in the transport experiments are out of equilibrium in many cases. Moreover, the state of the system may also be time dependent. These features make the investigations unaccessible from the conventional many-body tools. So an essentially exact numerical method for the non-equilibrium and time dependent phenomena in the interacting nano-devices is highly desirable, which can also verify the approximations used in various analytical approaches.

There exist several powerful methods to deal with the low dimensional correlated systems, such as the numerical renormalization group (NRG) and the density-matrix renormalization group (DMRG). With the input from the quantum information science, time-evolving block decimation (TEBD)⁷ ⁸ and adaptive time dependent DMRG (t-DMRG) have received much attention.⁹ ¹⁰ To our knowledge, there are some previous studies of the non-equilibrium transport of the nano-devices using the adaptive t-DMRG technique.¹¹ ¹³ By adopting the logarithmic discretization, da Silva et al. ¹⁴ have studied the Kondo correlations. Guo et al. ¹⁵ have examined the noninteracting resonant level model in the Landau-Zener potentials. Besides the adaptive tDMRG approach, there are also attempts based on the time-dependent NRG ¹⁶, functional RG ¹⁷, Dyson equation embedding ¹⁸, flow-equations ¹⁹ ²⁰, and quantum Monte Carlo ²¹ ²⁴ methods. But the adaptive t-DMRG approach gives direct access to the transient regime and could handle the time dependent Hamiltonian directly. The tVMPS approach adopted in this paper is directly connected with the adaptive t-DMRG ⁹ ¹⁰ and the TEBD ⁷ ⁸ approaches. The computational cost of these two methods is very similar, and in practice both methods achieve a similar accuracy. ²⁴

The merit of the VMPS approach lies in two aspects. First, it represents a large class of states, which could be seen from the success of the NRG and DMRG approaches (which generate MPS in their processes) for the zero and one-dimensional quantum models. And the fact that the entanglement entropy increases slowly in one dimension also permits one to simulate the states classically using the VMPS method. ²⁴ Second, it is easier to handle the MPS i.e., the overlap of two MPS, the expected value of an operator in a given MPS etc. can be calculated with polynomial complexity.

In this paper we study the spin current through an ESR quantum dot with Coulomb interaction ²⁵ ²⁷. We obtain the transient as well as the quasi-steady state spin current using the time-dependent VMPS method. We also studied the effect of the interacting on the spin current. The results are compared with time-dependent Hartree-Fock approximation (TD-HF) and non-equilibrium Green’s function (NEGF) approach for the quasi-steady state.
II. MODEL

We consider an ESR setup of a quantum dot, where single-electron level of the dot is split by the Zeeman field $B_0$ and the two spin levels are coupled by a rotating magnetic field $B_1$($\cos(\omega \tau), \sin(\omega \tau)$). The Hamiltonian reads $H = H_{\text{dot}} + H_{\text{rotate}} + H_{\text{lead}}$

$$H_{\text{dot}} = V_g \sum_\sigma n_\sigma \frac{g \mu_B B_0}{2} (n_\uparrow - n_\downarrow) + U n_\uparrow n_\downarrow$$

$$H_{\text{rotate}} = -\frac{g \mu_B B_1}{2} \sum_\sigma (d_\sigma^\dagger d_\sigma e^{i \omega \tau} + d_\sigma^\dagger d_\sigma e^{-i \omega \tau})$$

$$H_{\text{lead}} = -t' \sum_\sigma \sum_{i=1:|a|} (d_\sigma^\dagger c_{i,\sigma} + h.c.)$$

$$-t \sum_{\sigma} \sum_{i=1:|a|} (c_{i,\sigma}^\dagger c_{i+1,\sigma} + h.c.). \quad (1)$$

Here $d$ and $c$ denote the annihilation operator of electron in the dot and the lead. $H_{\text{lead}}$ contains the terms describing coupling of the dot with the lead and the hopping in the lead. $H_{\text{rotate}}$ contains the rotating magnetic field. $H_{\text{dot}}$ contains the Zeeman splitting, the gate voltage terms and the on site Coulomb repulsion between the spin up and down electrons. In the present study we fix $t = 1$ and $g \mu_B B_0 = \omega = 1$ where the ESR resonance condition is satisfied. We set $g \mu_B B_1 = 2$ and $t' = 0.4$ unless mentioned. The single lead is a noninteracting chain with $N_{\text{lead}}$ sites. The coupling of it with the QD is described by the hybridization $\Gamma = \pi t'^2 \rho$.

III. METHODS

The time dependence of the Hamilton could be eliminated by the unitary transformation $U = e^{-i(\omega \tau/2)\sum_\sigma (c_{i,\sigma}^\dagger c_{i,\sigma} + c_{i,\sigma} c_{i,\sigma}^\dagger)} + (d_\sigma^\dagger d_\sigma - d_\sigma d_\sigma^\dagger)$. It transforms the Hamiltonian into rotating reference frame (RF), see Fig.1(b). One can see that the rotating magnetic field, in effect, shifts electron energy to the opposite direction for up and down spins. Quasi-steady state spin current has been studied in the RF using the non-equilibrium Green’s function (NEGF) method in the noninteracting case and by NRG approach in adiabatic limit. In the following we will revisit the problem in transient as well as quasi-steady regime, and treat the interacting non-perturbatively with the exact numerical methods.

For the time dependent Hamiltonian $H(\tau)$, the evolution of the density matrix $\rho$ follows the von-Neumann equation $i \frac{d\rho}{d\tau} = [H, \rho]$. For the noninteracting case, one could write $H(\tau)$ with the single particle basis. Then direct integration of the von-Neumann equation with a given initial condition $\rho(\tau = 0) = \rho_0$ could be easily done. The initial density matrix $\rho_0$ is calculated in form ground state of the SIAM chain without the rotating magnetic field $B_1$.

From the density operator $\rho(\tau)$ the occupation on the dot is calculated by $n_\sigma(\tau) = \langle \psi(\tau)|d_\sigma^\dagger d_\sigma|\psi(\tau)\rangle$, and the spin current through the dot is $J^\sigma = \frac{\hbar}{\pi} \text{Im} \langle t' \langle \psi(\tau)| d_{\sigma}^\dagger c_{1,\sigma} |\psi(\tau)\rangle \rangle$, i.e. they are evaluated on the bond connect the dot and the lead. We set $g \mu_B = e = \hbar = 1$ in this paper.

For the interacting case we adopt the VMPS approach to calculate the ground state of $H(\tau = 0)$. Then we apply the rotational magnetic filed $B_1$ on the dot at $\tau = 0$, and
Figure 3: (color online) Dot occupancy for each spin (upper panel) and spin current (lower panel) for a 64 sites chain with different gate voltage. The shaded region is averaged to calculate the quasi-steady state spin current.

Perform the time evolution. To reduce the dimension of the local Hilbert space, an unfolded technique is used, the original SIAM chain is unfolded into two chains with different spins. The total length of the unfolded SIAM chain is \( L \). They are connected at the end point by the Coulomb repulsion and the rotating magnetic field \( B_1 \). The errors of the computation mainly come from the following sources. First the Trotter decomposition error. Second the truncation errors accumulated in the course of the time evolution. For short time scale the Trotter error dominates while for the long time the truncation error dominates. Caution must also be taken because of the finite size of the leads. The electrons may bounce at the end point and the spin current flows along the reverse direction. This is an artifact of the present method and could be eliminated by careful finite size scaling analysis.

We also use time-dependent Hartree-Fock (TD-HF) method to investigate the interacting case approximately, in which the interaction term is factorized into \( U(\langle n_\uparrow \rangle n_\downarrow + n_\downarrow \langle n_\uparrow \rangle) \). At each time step of the integration of the von-Neumann equation, the dot occupation which is used to update the Hartree-Fock Hamiltonian. This approach is as efficient as the non-interacting cases.

### IV. RESULTS

In Fig. 2 we show the development of the spin current after the rotational magnetic field \( B_1 \) is applied to the noninteracting dot. To reduce the transient region, we use a larger coupling constant \( t' = 1 \) here. For small chain length \( (L = 8, 16) \) the finite size effect shows up within the maximum time of our simulation. The charge pulse reaches the end of the chain and bounces back thus causes the reversing of the sign of the spin current. However, the spin current reaches a saturation value for larger chain length \( (L = 8, 16) \) which indicates the quasi-steady state spin transport is achieved. In the quasi-steady state, the spin up electrons flow in the dot, flip their spins and then flow away. There is no net charge transport since \( J_\uparrow = -J_\downarrow \). Overshooting behavior at short time scales \( (\tau \sim 1.8) \) is observed. It is due to abrupt applying of the rotational magnetic field and could be suppressed if the rotational magnetic field is turned on adiabatically. The tVMPS result for \( L = 32 \) nicely follows the direct integration of the von-Neumann equation. The oscillation at long times in the tVMPS approach was also noticed in the previous study with the adaptive t-DMRG approach [13]. With the increasing of the bond dimension, the oscillation tends to disappear. The coincidence validates the VMPS method for the noninteracting case. However, its main power lies in the interacting cases and we expect similar precision could be achieved in that case.

Electron occupation and spin current through the quantum dot are calculated as functions of time for different gate voltages \( V_g \), shown in Fig. 3. It is seen that the overall occupation on the dot oscillates as it reaches its quasi-steady-state value, the spin current develops in the mean time. Note that the transient state current can even be of the opposite sign with its value in the quasi-steady state, Fig. 3(b). By taking average of physical quantities in the quasi-steady state, we extract variation of the quasi-steady-state dot occupation and spin current with the gate voltage \( V_g \), see Fig. 3. The spin polarization in the steady state is less pronounced than the initial state. And it is even inverted for \(-1 < V_g < 1\), Fig. 3(a). The steady state current attains its maximum value at \( V_g = \pm 1 \). This is the case where \( n_\uparrow = n_\downarrow \), i.e. the dot is spin unpolarized. It can be seen from Fig. 3(b), in this case \( V_g \pm B_1 = 0 \) and the \( | \downarrow \rangle \rightarrow | \uparrow \rangle \) is tuned to zero energy point. Spin flip process on the dot is most efficient and gives a maximum spin current. We also use NEGF to study the current and occupation in the RF, see inset of Fig. 3(a). It gives qualitatively similar results, the small discrepancy is due to the finite size effect of the tVMPS approach. It should be noted that NEGF approach adopted here does not yield results of transient state since the unitary transformation eliminates the time dependence. To take into account the initial condition properly, the two-time Green’s function should be used [30, 32].

For interacting case, we calculate the real time spin current through the ESR-QD by tVMPS method. The results were compared with TD-HF results, see Fig. 4 for \( U = 1 \). Although there are discrepancies in the real time data, the TD-HF approximation captures the overall behavior of the spin current. This is due to the Kondo physics—which is missing from the TD-HF approach—does not manifests itself here since the presence of large magnetic field \( B_1 \) and Fermi surface splitting in the lead. Kondo effect may restored when \( B_1 \) is reduced below Kondo temperature [27]. But small \( B_1 \) also reduce the
chance of spin flip process on the QD, thus reduce the spin current through it. Surprisingly, the average of physical quantities in the quasi-steady state of these two approaches are in good agreement, see Fig. 5. Based on this investigation, we validate that the HFA is a good approximation for the qualitative investigation of spin-pump devices away from the Kondo regime. However, caution must be taken when it is used to make prediction on the real time dynamics. For example for the \( V_g = -1.0 \) case, the transient state spin current of TD-HF is of the opposite sign to the tVMPS prediction, thus it is quantitative wrong.

The magnitude of spin current with the gate voltage is still a two-peaked curve similar to the noninteracting case. Interaction has different effects on the high and low filling regimes of the dot, Fig. 4 (b). It does not modify the dot occupation and the spin current dramatically for \( V_g > 0 \). The peak of the spin current remains at \( V_g = 1 \) and the maximum value is only suppressed by one percent up to \( U = 3 \). However, since the average dot occupation is larger than 1 for \( V_g < 0 \), the correlation effect shifts the spin current peak downwards by \( U \). This is a manifestation of the Coulomb blockade effect.

The fluctuation of the density \( \Delta = \langle \delta n_\uparrow \delta n_\downarrow \rangle = \langle n_\uparrow n_\downarrow \rangle - \langle n_\uparrow \rangle \langle n_\downarrow \rangle \) is also calculated. It is a measure of the accuracy of the HF approach. This quantity is conserved under the particle-hole transformation. Thus two different gate voltages satisfying \( V_g + V_g' = -U \) give the same value of \( \Delta \). This is respected in the tVMPS calculation. But the discrepancy from the tVMPS is unrelated to it, \( i.e. \), although \( V_g = 1 \) and \( V_g = 0 \) has the same \( \Delta \), the discrepancy of the spin current from the tVMPS result is not the same. We find the HF approximation is surprisingly good for the quasi-steady state physical quantities even if the fluctuation is relatively large. The fluctuation is always negative due to the Cauchy-Schwarz inequality, indicating that the HFA overestimates the potential energy. The absolute value of the fluctuation reaches its maximum 0.2 for \( -1 < V_g < 0 \). However, even for these cases, the HF data still shows good agreement with the tVMPS data.

V. CONCLUSION

To conclude, we perform essentially exact real time calculation of the spin current through an interacting ESR quantum dot. We benchmark the essentially exact tDMRG result against those from various analytical and approximate methods. From the extracted average spin current, we obtain the Coulomb block shift of the spin current peak, confirmed by the time-dependent Hartree-Fock calculations. We find that the spin current attains its maximum for a spin neutral quantum dot. The spin neutral condition is fulfilled for two gate voltages \( V_g = 0 \) and \( V_g = 1 \), where the absolute values of the fluctuation are maximum.

The two spin current peaks respond differently to the electronic correlation, the lower filling peak is nearly unaffected. Comparison to the NEGF approach with an infinite lead shows that the finite size effect does not affect the qualitative behavior of the quasi-steady-state quantities. These results are also compared with those of the TD-HF approach. It is shown that the TD-HF gives accurate quasi-steady-state dot occupation and
spin current. However its prediction on the real time
dynamics is problematic.

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