J. At. Mol. Sci.
doi: 10.4208/jams.062111.081811a

Vol. **3**, No. 3, pp. 244-251
August 2012

Phonon-assisted spin current in a hybrid system with a single molecular quantum dot system applied with ac magnetic fields

Qiao Chen*

Department of Maths and Physics, Hunan Institute of Engineering, Xiangtan 411104, China
Received 21 June 2011; Accepted (in revised version) 18 August 2011
Published Online 18 February 2012

Abstract. We investigate the spin current through a molecular quantum dot (MQD) irradiated with a rotating magnetic field and an oscillating magnetic field by nonequilibrium Green's function. The rotating magnetic field rotates with the angular frequency ω_r around the z-axis with the tilt angle θ, and the time-oscillating magnetic field is located in the z-axis with the angular frequency ω. Different behaviors have been shown in the presence of electron-phonon interaction(EPI) which plays a significant role in the transport. The spin current displays asymmetric behavior as the source-drain bias $eV=0$, novel side peaks or shoulders can be found due to the phonon absorption and emission procedure, and the negative spin current becomes stronger as the parameter g increases. However, the spin currents display the same magnitude and the same oscillation behavior in the region $\mu_0 B_1 > 3\Delta$ regardless the parameter g.

PACS: 74.50.+r, 73.40.-c, 73.21.-b, 72.10.Bg

Key words: molecular quantum dot, spin-flip effect, electron-phonon interaction, nonequilibrium Green's function

1 Introduction

The manipulation of spin is one of the fundamental processes in spintronics, providing the possibility of writing information in a magnetic memory [1], and also because of the possibility of classical or quantum computation using spin. Usually the effect of spin is very small in non-magnetic materials, and it can be neglected in the absence of magnetic field. However, the spin of an electron is responded to an applied magnetic field sensitively. Recently, many efforts have been made to this area. Datta and Das have made

*Corresponding author. *Email address:* `cqhy1127@yahoo.com.cn` (Qiao Chen)

the pioneering contribution to the exploration of spin-dependent semiconducting nanodevice [2]. In this structure, the current arises from the spin precession due to spin-orbit coupling in narrow-gap semiconductor. The theoretical work of efficient spin filter has been discussed based on a quantum dot (QD) in the Coulomb blockade regime weakly coupled to leads [3]. The spin-current circuit and generator phenomena are also proposed to design spin-battery [4–6]. The Rashba term affects the transport in nonmagnetic resonant tunneling diode [7]. Therefore a very prosperous frontier of investigation known as spintronics is developing correspondingly. The dissipatedness spin transport [8], quantized spin conductance in insulating system provide some examples of spintronics [9]. Spin-flip transport through a quantum dot system also has been discussed [10].

The study of electronic transport through molecular devices has attracted considerable attention [11–14]. Molecular devices consist of single molecules connected to leads, where vibrations and electronic interactions operate [11]. The experiments show that the electron-phonon interaction(EPI) becomes more and more important in electronic transport through a very small single molecular device [11]. As a tunneling electron travels through a MQD, if its residence time on the MQD can be compared with the time of nuclear vibration, the inelastic tunneling will have a great impact on electron transport properties. It was first observed in a single C_{60} molecule that the signs of vibrational sidebands were shown in transport [11, 15–17]. Many other molecules can also be taken as MQDs, such as carbon nanotubes [18], octanethiols [19], ultrasmall metallic particles [20], and other self-assembling organic molecules [21]. Theoretically, many efforts have been made toward quantum transport through MQDs system, such as kinetic equation approach [22], the rate equation approach [23], the nonequilibrium quantum theory [24, 25] and the numerical renormalization group calculation [26, 27]. This paper is contributed to the MQD system under the perturbation of a rotating magnetic field and an oscillating magnetic field, where the spin current is modified due to the EPI. We derive the spin current formula first, and then perform the numerical calculation.

2 Model and formalism

We consider the circumstance that a MQD is coupled to two metallic leads. Only single level MQD without inter- or intradot Coulomb interactions are considered, which is coupled to the local vibration mode and irradiated with a rotating magnetic field and an oscillating magnetic field. The rotating magnetic field rotates with the angular frequency ω_r around the z-axis with the tilt angle θ, and the azimuthal angle $\varphi(t)=\omega_r t$, i. e. , $\mathbf{B}_0(t)=\mathbf{B}_0(\sin\theta\cos\varphi(t))\mathbf{e}_x+\sin\theta\sin\varphi(t))\mathbf{e}_y+\cos\theta\mathbf{e}_z)$. The time-oscillating magnetic field $\mathbf{B}_1(t)$ located in the z-axis is defined as $\mathbf{B}_1(t)=B_1\cos(\omega t)\mathbf{e}_z$, where ω is the angular frequency of the oscillating magnetic field. The total magnetic field applied to the MQD