Spin-dependent thermal and electrical transport in a spin-valve system

Zheng-Chuan Wang,[1] Gang Su,[1,2,*] and Song Gao[2]
[1]Department of Physics, Graduate School, Chinese Academy of Sciences, P.O. Box 3908, Beijing 100039, China
[2]State Key Laboratory of Rare Earth Materials Chemistry and Applications, PKU-HKU Joint Laboratory on Rare Earth Materials and Bioinorganic Chemistry, Peking University, Beijing 100871, China

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Within the framework of Büttiker's gauge invariant and charge conservation dc transport theory, the spin-dependent thermal and electrical transport in a ferromagnet-insulator-ferromagnet tunnel junction is investigated at finite bias voltage and finite temperature. It is observed that the relative orientations of magnetizations in the two ferromagnetic (FM) electrodes as well as temperature have remarkable effects on the differential conductance, thermopower, Peltier effect, and thermal conductivity. At low temperature the quantum resonant tunneling is predominant, leading to the deviation of classical transport theory, while the transport of electrons are crucially governed by thermal processes at high temperature. The so-called spin-valve phenomenon is clearly uncovered for both the differential conductance and the thermal conductivity at low temperature. The Wiedemann-Franz law is examined, and the inelastic tunneling spectroscopy is also discussed. Our findings are expected to be measured in the near future.

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I. INTRODUCTION

During the past decade, the thermal and electrical transport in various microstructures, an important yet fundamental question in mesoscopic systems (see, e.g., Ref. 1), has been intensively explored both experimentally and theoretically. Among others, the quantum oscillations of the thermopower, the quantum size effect on the thermal conductance and the Peltier coefficient,[2] the diffusive thermopower in the Coulomb blockade nonlinear regime,[3] and so on, have been successfully measured for a quantum point contact. There are also a lot of measurements done concerning the thermoelectric transport properties in quantum wires and other two-terminal structures. Experimental results show that the quantum-mechanical principles and the size effect play an essential role in the transport in microstructures at low temperatures.

Theoretically, a multichannel Landauer formula for the thermoelectric transport when studying the thermopower near the mobility edge has been derived,[4] which was later extended to account for the case when temperature changes in the reservoirs and heat flux in the terminals, where the thermoelectric transport coefficients are given in terms of the scattering matrix of the microstructure.[5] Based on Büttiker's formalism proposed for the dynamic conductance,[6–8] which guarantees the current conservation and the gauge invariance by taking the contributions of displacement current originated from electron-electron interactions into account, the dc and ac low frequency linear and weak nonlinear thermoelectric response in a multiprobe mesoscopic system were studied.[9] Despite all that, direct calculations of the spin-dependent thermoelectric transport in ferromagnetic tunnel junctions, to our knowledge, are still sparse, as the recent experimental studies on spin tunneling in ferromagnetic junctions have yielded a plenty of results and applications (see Refs. 10 and 11 for excellent reviews). It is therefore quite necessary to pay attention to this intriguing microstructure.

It is the purpose of this paper to present a direct calculation on thermal and electrical transport properties such as the differential conductance, the thermopower, the Peltier coefficient, the thermal conductivity as well as the inelastic tunneling (IET) spectra of a spin-valve system within the framework of Büttiker's gauge invariant and current conservation formalism. As is known, a spin valve is formed when two ferromagnetic conductors are separated by an insulating or semiconducting barrier. Such a system was first established when studying the spin-polarized electrons in ferromagnets tunneling across an insulator barrier by Meservey and Tedrow,[12] and then the relative orientation of the magnetizations of left and right ferromagnetic electrodes dependent tunneling, was observed by Jullière[13] and subsequently by Maekawa and Gäfvert,[14] and the junction magnetoresistance (JMR) in ferromagnet-insulator(semiconductor)-ferromagnet [FM-I(S)-FM] junctions was measured. Recently, a large JMR was obtained at room temperature in FM-Al_2O_3-FM junctions.[15] Jullière was first to give a simple model based on the classical tunneling theory to predict the existence of a large JMR in FM-I-FM films.[13] By considering the barrier and the electrodes as a quantum mechanical system, Slonczewski developed a theory on the electrical conductance of a magnetic valve.[16] The tunneling magnetoresistance (TMR) was analyzed by Bratkovsky[17] for ferromagnet-insulator-ferromagnet junctions, including half-metallic systems. There are also some approaches based on the linear-response theory and Landauer formula for spin-valve systems; see Ref. 11 for a review. In this paper, we shall present a thermoelectrical transport theory to study the bias voltage and temperature dependences of thermal and electrical transport properties for FM-I(S)-FM junctions on the basis of the framework of Büttiker's current conservation and gauge invariance formalism which has been successfully applied to a few interesting mesoscopic systems.[18] Since there are few experimental measurements appeared in literature on the thermoelectric transport quantities of the ferromagnetic tunnel junctions, we expect that our calculated results would be tested in realistic systems.

The outline of this paper is arranged as follows. In Sec. II, a general formalism for the thermal and electrical transport quantities at finite bias voltage will be presented. In Sec. III, the dependences of the differential conductance, thermopower, Peltier effect, thermal conductivity, and IET spectroscopy on the bias voltage and the relative orientations of magnetizations between the two ferromagnetic electrodes at finite temperatures will be investigated. The Wiedemann-Franz law will also be examined. Finally, a summary and discussion of our results will be given.

II. GENERAL FORMALISM

Consider a spin valve [i.e., a FM/I(S)/FM junction] which is connected by two reservoirs at contacts α $(=1,2)$ with the chemical potential μ_α. It is presumed that the thermalization of electrons by inelastic scattering and the Joule energy dissipation happen only outside the system but not inside. For the sake of simplicity, in the following we suppose that the bias voltage is very slowly tuned onto the system, and the temperature gradient along the junction is not so large. The transport properties of the system are described by the scattering matrix $S_{\alpha s,\beta s'}$ which relates the outgoing current amplitude at contact α with spin s to the incident current amplitude at contact β with spin s'. We start by writing down the electric current through contact α as[6–8]

$$I_\alpha=\frac{e}{h}\sum_{\beta=1}^{N}\int dE f_\beta(E-\mu_\beta)\sum_{s,s'}A_{\alpha s,\beta s'}(E), \tag{1}$$

where $f_\beta(z)=[1+\exp(z/k_BT_\beta)]^{-1}$ is the Fermi function, $A_{\alpha s,\beta s'}(E)=\delta_{\alpha\beta}\delta_{ss'}-S^{+}_{\alpha s,\beta s'}(E)S_{\alpha s,\beta s'}(E)$, $\mu_\beta=\mu+eV_\beta$, and $T_\beta=T+\theta_\beta$. When $\beta=1$, we have $\mu_1=\mu$ and $T_1=T$. The thermal current flowing towards the junction through contact α may be obtained by

$$Q_\alpha=\frac{1}{h}\sum_{\beta=1}^{N}\int dE(E-\mu_\beta)f_\beta(E-\mu_\beta)\sum_{s,s'}A_{\alpha s,\beta s'}(E). \tag{2}$$

In analogy to the bulk solids, the electric current **I**, and the energy current **Q**, can be *formally* expressed as[5]

$$\mathbf{I}=\mathbf{G}\cdot\mathbf{V}+\mathbf{L}\cdot\boldsymbol{\theta}, \tag{3}$$

$$\mathbf{Q}=\mathbf{M}\cdot\mathbf{V}+\mathbf{N}\cdot\boldsymbol{\theta}, \tag{4}$$

where **G**, **L**, **M**, and **N** are tensors, with matrix elements being $G_{\alpha\beta}$, $L_{\alpha\beta}$, $M_{\alpha\beta}$, and $N_{\alpha\beta}$, respectively. It is seen that the contributions to the electric and energy currents come from two processes, namely one from transport of electrons driven by the difference of the chemical potentials between the two electrodes and the other from the diffusive motion of electrons driven by the temperature gradient between the two electrodes, thereby leading to each current comprised of two parts. Consequently, the thermoelectric transport properties of microstructures such as spin valves can be investigated based on these two equations. The differential conductance, **G**, is defined as the derivative of the electrical current with respect to the bias voltage. The thermopower, **S**, is defined as usual as

$$\mathbf{S}=-\mathbf{G}^{-1}\mathbf{L}. \tag{5}$$

The Peltier coefficient, labeled by $\boldsymbol{\pi}$, and the thermal conductivity $\boldsymbol{\kappa}$, are defined by

$$\boldsymbol{\pi}=\mathbf{M}\mathbf{G}^{-1} \tag{6}$$

and

$$\boldsymbol{\kappa}=\mathbf{M}\mathbf{G}^{-1}\mathbf{L}-\mathbf{N}, \tag{7}$$

respectively. It is noteworthy that the differential conductance, thermopower, Peltier coefficient, and thermal conductivity, as defined above, are *formally* the same as those in bulk solids. In terms of Eq. (1), the differential conductance **G** can be found to be

$$G_{\alpha\beta}=\frac{e}{h}\sum_{\delta=1}^{N}\int dE\left[\left(\frac{\partial f_\delta(E-\mu_\delta)}{\partial V_\beta}\right)\sum_{s,s'}A_{\alpha s,\delta s'}(E)\,\delta_{\beta\delta}+f_\delta(E-\mu_\delta)\sum_{s,s'}\int dx\,\frac{\partial A_{\alpha s,\delta s'}(E)}{\partial eU(x)}u_\beta(x)\right], \tag{8}$$

where $\delta A_{\alpha s,\beta s'}/\delta eU(x)=-(S^{\dagger}_{\alpha s,\beta s'}[\delta S_{\alpha s,\beta s'}/\delta eU(x)]+[\delta S^{\dagger}_{\alpha s,\beta s'}/\delta eU(x)]S_{\alpha s,\beta s'})$, and $U(x)$ is the electrostatic potential. The characteristic potential $u_\alpha(x)$, defined by $dU(x)=u_\alpha(x)dV_\alpha$, satisfies the Poisson equation[6]

$$-\partial_{xx}u_\alpha(x)+4\pi e^2\int dx'\,\Pi(x,x')u_\alpha(x')=4\pi e^2\frac{dn_\alpha(x)}{dE}, \tag{9}$$

where $dn_\alpha(x)/dE=-(1/4\pi i)\Sigma_{\beta st}(S^{\dagger}_{\alpha s,\beta t}[\delta S_{\alpha s,\beta t}/\delta U(x)]-[\delta S^{\dagger}_{\alpha s,\beta t}/\delta U(x)]S_{\alpha s,\beta t})$, is the injectivity, characterizing the partial local density of states at contact α. The Lindhard polarization function $\Pi(x,x')$, in the Thomas-Fermi linear screening model, is the sum of local density of states $\Pi(x,x')=\Sigma_\alpha[dn_\alpha(x)/dE]\delta(x-x')$. To compute $\delta A_{\alpha s,\beta s'}(E)/\delta eU(x)$, we use the Fisher-Lee relation and the fact

$$\frac{\delta S_{ss'}(x_\alpha,x_\beta)}{\delta U(x)}=i\sqrt{v_\alpha v_\beta}\sum_m G_{sm}(x_\alpha,x)G_{ms'}(x,x_\beta),$$

in which $v=(1/\hbar)(\partial E/\partial k)$, and k is the wave vector. We would like to point out here that Eq. (8) justifies the differential conductance at finite bias voltage and at finite temperature. If one sets the bias $V_\beta=0$, by the current conservation relation $\Sigma_{\beta s'}A_{\alpha s,\beta s'}(E)=0$, the second term of the right-hand side of Eq. (8) is identically zero, while the first term is nothing but the dc *linear* conductance given by Büttiker. One may notice that although the first term also includes the bias voltage V_β, which originates from the contribution of the direct injected charge, the second term is from the contribution of electron-electron interactions, which contains the characteristic potential that describes the variation of the internal potential landscape due to a change of the electrochemical potential at contacts and is determined by the Poisson equation. It is this electron-electron interaction that induces the internal potential. The differential conductance at finite bias voltage should include contributions both from the first term and from the second term.

In the similar spirit and physical reasons, we find that the tensors **L**, **M**, and **N**, which are related to the thermoelectric transport properties through Eqs. (5), (6), and (7), take the following forms:

$$L_{\alpha\beta}=\frac{e}{h}\sum_{\delta=1}^{N}\int dE\Bigg[\left(-\frac{E-\mu_\beta}{T+\theta_\beta}\right)\partial_E f_\delta\sum_{s,s'}A_{\alpha s,\delta s'}(E)+f_\delta(E-\mu_\delta)\sum_{s,s'}\frac{1}{e}\left(\frac{E-\mu_\beta}{T+\theta_\beta}\right)\times\int dx\,\frac{\partial A_{\alpha s,\delta s'}(E)}{\partial eU(x)}u_\beta(x)\Bigg], \tag{10}$$

$$M_{\alpha\beta}=\frac{1}{h}\sum_{\delta=1}^{N}\int dE\Bigg[(E-\mu_\delta)\times\left(\frac{\partial f_\delta(E-\mu_\delta)}{\partial V_\beta}\right)\sum_{s,s'}A_{\alpha s,\delta s'}(E)\,\delta_{\beta\delta}+f_\delta(E-\mu_\delta)\sum_{s,s'}\int dx\,\frac{\partial A_{\alpha s,\delta s'}(E)}{\partial eU(x)}u_\beta(x)\Bigg], \tag{11}$$

and

$$N_{\alpha\beta}=\frac{1}{h}\sum_{\delta=1}^{N}\int dE\Bigg[(E-\mu_\delta)\left(\frac{\partial f_\delta(E-\mu_\delta)}{\partial\theta_\beta}\right)\delta_{\beta\delta}\times\sum_{s,s'}A_{\alpha s,\delta s'}(E)+f_\delta(E-\mu_\delta)\times\sum_{s,s'}\left(\frac{E-\mu_\beta}{T+\theta_\beta}\right)\int dx\,\frac{\partial A_{\alpha s,\delta s'}(E)}{\partial eU(x)}u_\beta(x)\Bigg], \tag{12}$$

where the notions are the same as in Eq. (8). The IET spectroscopy $G_{\alpha\beta\gamma}$, which is usually defined as the second derivative of the electrical current with respect to the bias voltage,[15] is also quite crucial of importance. It can be measured experimentally, as done for a few FM-I(S)-FM junctions. Based on above equations and analyses, we obtain

$$G_{\alpha\beta\gamma}=\frac{e}{h}\sum_{\delta=1}^{N}\int dE\Bigg[\left(\frac{\partial^2 f_\delta(E-E_F-eV_\delta)}{\partial V_\beta\partial V_\gamma}\right)\sum_{s,s'}A_{\alpha s,\delta s'}(E)\,\delta_{\beta\delta}\delta_{\gamma\delta}+\sum_{s,s'}\frac{\partial f_\delta(E-E_F-eV_\delta)}{\partial V_\beta}\int dx\,\frac{\partial A_{\alpha s,\delta s'}(E)}{\partial eU(x)}u_\gamma(x)\,\delta_{\beta\delta}+\sum_{s,s'}\frac{\partial f_\delta(E-E_F-eV_\delta)}{\partial V_\gamma}\int dx\,\frac{\partial A_{\alpha s,\delta s'}(E)}{\partial eU(x)}u_\beta(x)\,\delta_{\gamma\delta}+\sum_{s,s'}f_\delta(E-E_F-eV_\delta)\left(\int\frac{\partial^2 A_{\alpha s,\delta s'}(E)}{\partial eU(x_1)\partial eU(x_2)}u_\beta u_\gamma dx_1dx_2+\int\frac{\partial A_{\alpha s,\delta s'}(E)}{\partial eU(x_1)}u_{\beta\gamma}dx_1\right)\Bigg], \tag{13}$$

where $u_{\beta\gamma}$ is the second-order characteristic potential tentor, defined as $u_{\beta\gamma}=\partial^2U(x)/\partial V_\beta\partial V_\gamma$, satisfying

$$-\partial_{xx}^2u_{\beta\gamma}+4\pi e^2\frac{dn}{dE}u_{\beta\gamma}=4\pi e^2\left(\frac{d^2n_\beta}{dE^2}\delta_{\beta\gamma}-\frac{d^2n_\gamma}{dE^2}u_\beta-\frac{d^2n_\beta}{dE^2}u_\gamma+\frac{d^2n}{dE^2}u_\beta u_\gamma\right).$$

In comparison to the second-order weakly nonlinear coefficient of the dynamic conductance at zero bias, this above formula for finite bias voltages includes terms associated with the second-order characteristic potential and the second-order variation of $A_{\alpha s,\beta s'}(E)$. If the bias $V_\beta=0$, the last term in Eq. (13) is identically zero, and Eq. (13) recovers the dc second-order weakly nonlinear coefficient. It is worthwhile to emphasize that the first term comes from the direct injected charge, while the rest comes from the contributions from electron-electron interactions, manifested by the first-order and second-order characteristic potential.

Equations (1)–(13) comprise of the general formalism for the spin-dependent thermal and electrical transport properties of a spin-valve system at finite bias voltage and at finite temperature. Consequently, for a given model, if the scattering matrices or Green's functions of the system are gained within certain approximations, the thermal and electrical transport quantities can in principle be obtained. We would like to mention that these equations, with properly slight modifications, can also be applicable to studying the thermoelectric transport properties of various microstructures with multiterminals in mesoscopic scales.

III. THERMAL AND ELECTRICAL TRANSPORT PROPERTIES

Now, let us apply the general formalism developed in the preceding section to a specific model, i.e., a spin-valve system, to investigate the corresponding thermal and electrical transport properties at finite temperatures. As mentioned before, to calculate Green's function appeared in the foregoing equations, we assume a tight-binding model for ferromagnetic conducting layers for simplicity. Then, Green's function with spin can be formally expressed as $G=(E-H_c-\Sigma)^{-1}$, where H_c represents the Hamiltonian of the isolated system,[19] which involves with the electric potential in the insulator and the molecular fields in ferromagnets. The tight-binding dispersion relation is supposed to be $\varepsilon_{k_{\uparrow,\downarrow}}=2t(1-\cos k_{\uparrow,\downarrow}a)$ and $t=\hbar^2/2ma^2$, where we denote $k_{\uparrow,\downarrow}$ as wave vectors in the leads. If the spin polarization directions in two leads differ by an angle θ, the self-energies Σ_1 and Σ_2, which originate from the influence of the leads and only have contributions at the contacts, take forms of

$$\Sigma_1=\begin{pmatrix} -t\exp(ik_\uparrow a) & 0 \\ 0 & -t\exp(ik_\downarrow a)\end{pmatrix}, \quad \Sigma_2=\Re\Sigma_1\Re^\dagger, \tag{14}$$

where the rotation matrix $\Re$ is

$$\Re=\begin{pmatrix} \cos(\theta/2) & \sin(\theta/2) \\ -\sin(\theta/2) & \cos(\theta/2)\end{pmatrix}. \tag{15}$$

In our practical calculation, the molecular fields in the leads are assumed to be zero so as to simplify the self-energy terms. Here we would like to point out that although the bias dependence of the transport quantities should be in principle calculated by means of the nonequilibrium Green's function, we have supposed that the bias voltage and temperature are slowly added to the junction and the temperature gradient is quite small so that we can obtain the thermoelectric transport properties for not so large bias voltage and temperature gradient by invoking the equilibrium Green's function. This can be in some sense viewed as an approximation. Since this present paper is based on Buttiker's scattering matrix theory which is suitable for near-equilibrium system, our assumption of equilibrium instead of nonequilibrium Green′s function is reasonable. However, we would like to mention that this approximation has its limitations. It is suited to the case in low frequency ac fields and in small bias voltage. Besides, the bias voltage should be slowly added to the junction, otherwise it violates the near-equilibrium condition. Within the low frequency and small bias case, this approximation will not cause major changes in our prediction. The work based on the nonequilibrium Green's function is under way.

In the next subsections, we shall report our calculated results of the thermoelectric transport quantities using the formalism developed above for a FM/I(S)/FM single junction. For simplicity, we shall neglect the difference of the effective masses of electrons between in barriers and in ferromagnets, and treat them as the bare electron mass m_e. Though the ignorance of difference of effective masses in different layers would sometimes bring about negative polarization,[17] within our framework we find that this simplification would not cause a qualitative change in results. In the following we shall take $2m_e=e=k_B=\hbar=1$. The system consists of left and right two FM layers with width 2.0 nm and 6.0 nm, respectively, and an insulating (or semiconducting) layer with thickness 4.0 nm between the two FM conducting layers. The magnitude of the molecular field, $\mathbf{h}_0$, associated with the left and right FM layers are assumed to be 13.0 Ry and 8.0 Ry, and the barrier height in the insulator is supposed to be 0.02 Ry which is a convenient choice for our purpose and can be of course taken larger. This is an asymmetric junction. In order to ensure the validity of results, we have numerically checked the unitary properties of the scattering matrix as well as the consistency of the total density of states from two methods, namely the current conservation and the gauge invariance condition.

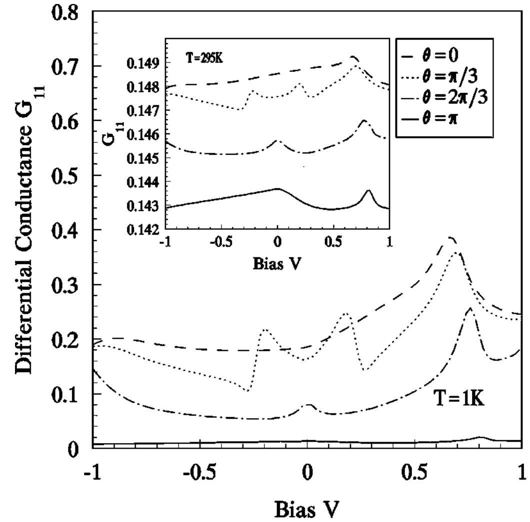

FIG. 1. The differential conductance (G) versus bias voltage at 1 K for different polarization directions. Shown in the inset is for the case at 295 K.

A. Differential conductance

The results for the differential conductance ($G\equiv G_{11}$) as a function of bias voltage for different polarization directions at two temperatures 1.0 and 295 K are presented in Fig. 1. At 1.0 K, we find that when $\theta=0$, the differential conductance is the biggest (besides small oscillations when $\theta=\pi/3$), and when $\theta=\pi$, the conductance eventually becomes vanishingly small however. This observation shows that the parallel polarization in the two FM layers makes electrons easy to tunnel, while the antiparallel polarization inhibits electrons to transmit, clearly suggesting a *spin-valve* effect. Here we reproduced this remarkable effect proposed by Jullière twenty-five years ago[13] based on a more general formalism. The underlying mechanism for it comes from the spin conservation during tunneling, as assumed by Jullière[13] and Slonczewski,[16] namely, the electrons with spin up and spin down tunnel through the barrier in the junction independently, and the tunneling currents flow in corresponding spin up and spin down channels. When spin polarizations in the two FM layers are parallel (e.g., aligning up), giving rise to the current flowing the biggest, while if the polarizations are antiparallel (e.g., aligning up in the first FM layer and down in the second FM layer), then a vanishingly small conductance is observed. Here we should point out that although for antiparallel alignment of magnetization there is a current flow experimentally observed for usual FMs, this could be caused by incomplete alignments of magnetizations in the incident FM layer, while in our calculation we have assumed that the incident FM layer is fully polarized (i.e., aligning up), leading to a small current flow observed. When θ is changing from 0 and π, the magnitudes of the conductance are decreasing, as seen from Fig. 1 with $\theta=\pi/3$ and $2\pi/3$ for examples. The bias-voltage dependence of the differential conductance are diverse for different angles θ, and the quantum oscillations appear at a few voltages. It deviates obviously from the classic ohmic law, namely, a few resonant peaks appear at some bias voltages. For example, at $\theta=\pi/3$ the resonant peaks appear at -0.2, 0.2, and 0.7 V, which manifests itself the quantum effect. The physical reason for this feature is that a proper combination of parameter values (e.g., the height and width of barrier in insulator and in FMs) forms a resonant structure, and at particular voltages the electrons overcome the barrier and take resonant tunneling, thereby resulting in the resonant peaks observed. For the set of parameter values assumed by us, around 0.7 V the electrons have energies comparable to the barrier height and thus easily transmit through the barrier, leading to a resonant peak occurring in the curve of the conductance regardless of the polarization direction (except for $\theta=\pi$). Our result indicates that at low temperature the conductance in a FM-I-FM junction is mainly governed by quantum tunneling processes, and the G-V relation no longer obeys the Ohmic law. Interestingly enough, such quantum resonant behaviors of the conductance at low temperatures in FM-I-FM junctions have been observed experimentally.[12,15] Our findings are qualitatively consistent with the experiments.

The situation changes when temperature is increasing. At intermediate temperature, the shapes of the G-V curves remain similar, but the quantum resonant peaks become blunt, and the magnitude of the conductance with bias voltage at $\theta=\pi$ become bigger. At higher temperature, an example of 295 K is shown in the inset of Fig. 1. From it we may see that the spin-valve effect disappears in this situation, and the conductance is almost independent of the bias voltage, albeit very small resonant peaks are seen, showing that at high temperature the spin polarization direction does not have remarkable effect on the conductance, and the antiparallel polarization makes only a few percent smaller than the parallel polarization. This observation implies that the conductance recovers the classic Ohmic law at high temperatures, indicating that it is not determined by the quantum tunneling process, but determined dominantly by the thermal activated and diffusive process. The fact that the spin-valve phenomenon cannot appear at high temperatures, is easily understood, because in this case the thermal fluctuations upset the spin alignments in the two FM electrodes and make spin flips, leading to spin up and spin down channels, despite perfect or partial perfect, are always connected through, causing the current flowing through the junction. As a result, the transport of electrons are primarily driven by the thermal process, leaving the conductance almost unchanged when the bias voltage is altered. Here we would like to mention that in some experiments the spin-valve effect in tunnel junctions can be observed even beyond 550 K. Since in our calculations we have adopted a simplified model and utilized some approximations, we have found that for our chosen parameter values which may be different from the realistic values assumed by experiments, the spin-valve effect disappears at 295 K, but this does not mean that our result is incompatible with experiments. Actually, as stated above, our result is qualitatively consistent with experimental observations.

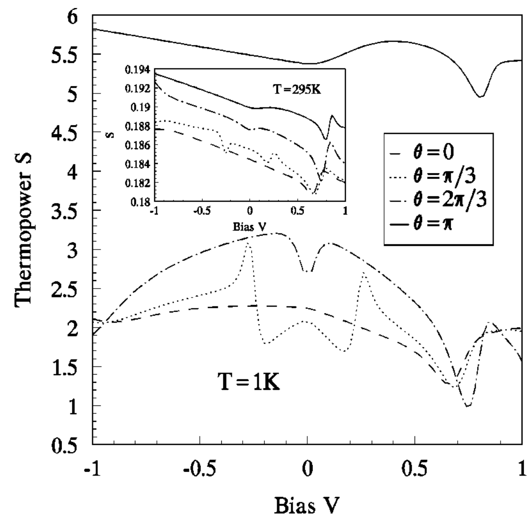

FIG. 2. The thermopower (S) versus bias voltage at 1 K for different polarization directions. Shown in the inset is for the case at 295 K.

B. Thermopower

The bias-voltage dependence of the thermopower ($S\equiv S_{11}$) for different angles of spin polarizations at finite temperatures are calculated, as shown in Fig. 2. At $T=1$ K, we may see that S exhibits quantum oscillations at certain voltages for different θ, showing the quantum tunneling process plays a considerable role in the thermoelectric transport of electrons at low temperatures. For θ varying from 0 to $2\pi/3$, the magnitudes of S, though a few resonant peaks existing, change not so much, while when $\theta=\pi$, S is obviously larger than the values at $\theta<2\pi/3$. This result indicates that the antiparallel spin polarizations of electrons enable the thermopower to be the strongest, which is certainly caused by the spin valve effect, because the thermopower is inversely proportional to the differential conductance which is vanishingly small in this case. When temperature is increasing, the shapes of the curves of S remain almost unaltered, but the magnitudes are decreasing. At high temperature, we have calculated S for different θ at $T=295$ K, as shown in the inset of Fig. 2. One can observe that regardless of few small resonant peaks the thermopower keeps almost unchanging with the bias voltage, and does not depend so much on the spin-polarization directions, suggesting again that at high temperature the thermoelectric transport of electrons in the

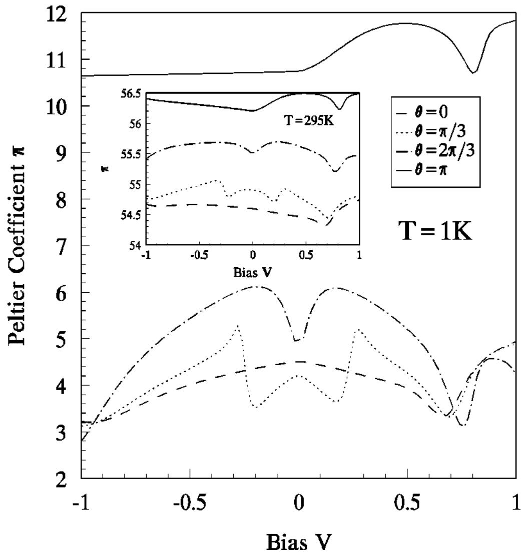

FIG. 3. The Peltier coefficient (π) versus bias voltage at 1 K for different polarization directions. Shown in the inset is for the case at 295 K.

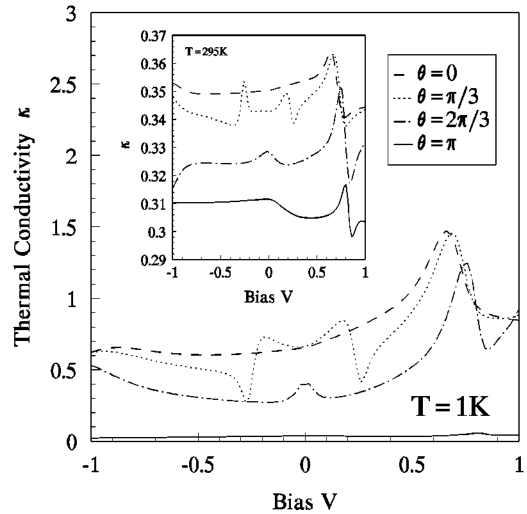

FIG. 4. The thermal conductivity (κ) versus bias voltage at 1 K for different polarization directions. Shown in the inset is for the case at 295 K.

spin-valve system is predominantly governed by thermal processes, and the classic results are recovered.

C. Peltier effect

Based upon the formalism presented in Sec. II, we have calculated the bias voltage dependence of the Peltier coefficient ($\pi \equiv \pi_{11}$) for different spin polarization directions at finite temperature, as shown in Fig. 3. At $T=1$ K, it can be seen that the Peltier coefficient has quantum oscillations at certain voltages for different θ, showing the quantum tunneling process plays a considerable role at low temperatures. As $\theta=0\sim 2\pi/3$, the magnitudes of the Peltier coefficient change not so much apart from a few resonant peaks, whereas at $\theta=\pi$, the Peltier coefficient is obviously larger than the values at $\theta<2\pi/3$, which indicates that the antiparallel spin polarizations of electrons enable the Peltier effect to be the strongest, which is closely related to the spin-valve effect, for the Peltier coefficient is inversely proportional to the differential conductance. At high temperature, we have uncovered that regardless of few small resonant peaks the Peltier coefficient keeps almost unchanging with the bias voltage, and also does not depend so much on the spin polarization directions, as shown in the inset of Fig. 3 at $T=295$ K for an example, which illustrates that the thermoelectric transport of electrons in this junction is predominantly governed by thermal processes at high temperature, and the magnitudes are greatly increasing compared with 1 K case while the shapes of the curves remain almost unvarying. It is worth noting that the curves shown in Figs. 2 and 3 for the thermopower and the Peltier coefficient look very alike, albeit the magnitudes between them differ. If one recalls the definitions of both, one may find this result is understandable, as the temperature gradient was assumed to be small in our calculations.

D. Thermal conductivity

Another important transport quantity, namely the thermal conductivity ($\kappa \equiv \kappa_{11}$), as a function of the bias voltage and the spin polarization directions at finite temperature, has been investigated. The calculated results are shown in Fig. 4. At $T=1$ K, the thermal conductivity displays a few resonant peaks with increasing the bias voltage for $\theta=0\sim 2\pi/3$, showing the thermal transport is primarily governed by the quantum tunneling process. When $\theta=\pi$, the thermal conductivity becomes vanishingly small, being a consequence of the spin-valve effect. The underlying reasoning for this phenomenon is the same as that explained when discussing the differential conductance. At high temperature, as shown in the inset of Fig. 4 for $T=295$ K as an example, the thermal conductivity varies only a few percent with the bias, and it does not depend much on the spin polarization directions of electrons in FM layers, suggesting the thermal effect plays a dominant role in the transport process in this situation. Once again, one may notice that the curves presented in Figs. 1 and 4 are very similar except for the diverse differences of magnitudes between them. The cause for this accidental fact may be resulted from the small temperature gradient assumed during our calculations. In a word, the thermal conductivity exhibits the qualitative similar behaviors as the differential conductance both at low and high temperatures in the present model.

It is known that in conventional metals the Wiedemann-Franz law, i.e., $\kappa/GT=L_0$ where L_0 is the Lorentz constant number, is obeyed. How about the situation in the spin-valve system? Let us now examine the quantity κ/GT as a function of the bias voltage and the spin polarization directions at finite temperature, and the results are presented in Fig. 5. It is seen that at low temperature (e.g., $T=1.0$ K) the ratio κ/GT slightly changes with the bias voltage, namely, when $\theta=0$ and π, it remains almost constant with the bias, but when $\theta=\pi/3$ and $2\pi/3$, it shows a few round peaks and dips. At $T=295$ K, this ratio varies with the bias only on the scale of

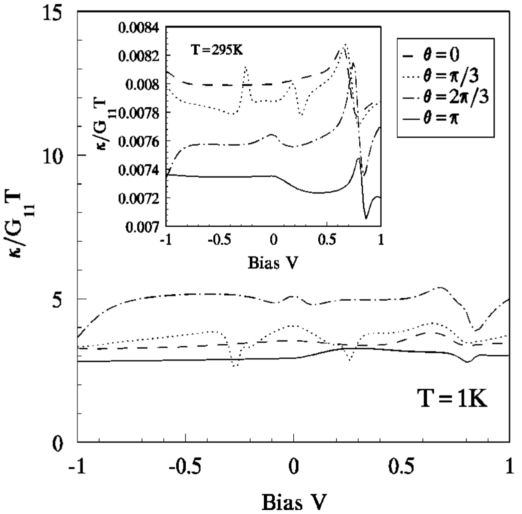

FIG. 5. The ratio κ/GT versus bias voltage at 1 K for different polarization directions. Shown in the inset is for the case at 295 K.

a few per ten mille, suggesting that it is almost unchanging. Within our approximations, κ/GT depends much weakly on the bias voltage and spin polarization directions in the two FM electrodes at finite temperature. However, this ratio changes drastically with temperature, i.e., it might decrease with increasing temperature. Consequently, the Wiedemann-Franz law is violated in this spin-valve system in the sense that the ratio κ/GT is no longer a constant number.

E. IET spectroscopy

The IET spectroscopy is usually defined as the derivative of the differential conductance with respect to the bias voltage, which can be measured in experiments. We have calculated it for the present spin valve system. The results of G_{111} as a function of bias voltage for different polarization directions are given in Fig. 6 at temperature 1 and 295 K, respectively. It is seen that the spectra depend on the spin polarization directions at a given temperature. For instance, at $T=1$ K, there are two peaks occurring for $\theta=0$, while there appear to be six peaks for $\theta=\pi/3$, and four peaks for $\theta=\pi$, as showed in Fig. 6. Away from the resonant regime, the background of the spectra $G_{111}(V)$ seems to decrease with increasing θ. At $\theta=\pi$, the background is almost vanishing. When temperature is increasing, apart from that the weights of some peaks have slight changes, the shape of the derivative of conductance as a function of bias voltage remains unchanged, showing that the IET spectra in FM/I(S)/FM junctions are *insensitive* to temperature. This character is qualitatively consistent with the experimental observation.[15] The inset of Fig. 6 is an example at $T=295$ K. Here we would like to point out that to simplify the calculation we have adopted a quasineutrality condition in the Poisson equation obeyed by the second-order characteristic potential $u_{\beta\gamma}$, resulting in

$$u_{\beta\gamma}=\left[\frac{d^2n_\beta}{dE^2}\delta_{\beta\gamma}-\frac{d^2n_\gamma}{dE^2}u_\beta-\frac{d^2n_\beta}{dE^2}u_\gamma+\frac{d^2n}{dE^2}u_\beta u_\gamma\right]\Big/\frac{dn}{dE},$$

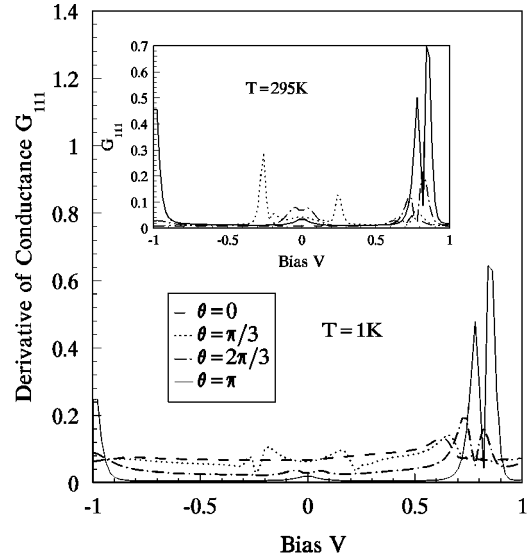

FIG. 6. The IET spectroscopy (G_{111}) versus bias voltage at 1 K for different polarization directions. Shown in the inset is for the case at 295 K.

which implies that the polarization charge has been omitted. Besides, in order to make clear which contribution is dominant in $G_{111}(V)$ spectra, we have calculated separately the contributions from direct injected charges and from electron-electron interactions, and found that the contribution from electron-electron interactions dominates.

IV. SUMMARY AND DISCUSSION

To summarize, we have extended Büttiker's gauge invariant and charge conserving dc transport theory to a spin-valve system at finite bias voltage and finite temperature for the first time. Within a tight-binding model, the electrical and thermal transport properties of the magnetic junction system, including the differential conductance, thermopower, Peltier effect, thermal conductivity, and IET spectroscopy, are calculated. It has been observed that the relative orientations of magnetizations in the two ferromagnetic electrodes as well as temperature have remarkable effects on the electrical and thermal transport properties. At low temperature the quantum resonant tunneling is predominant, leading to the deviation of classical transport theory, while the transport of electrons are crucially governed by thermal processes at high temperature. The so-called spin-valve phenomenon is clearly uncovered for both the differential conductance and the thermal conductivity at low temperature, namely, the parallel orientation of magnetizations in the two FM electrodes makes the maximal electrical and thermal currents observed, while the antiparallel orientation inhibits electrons from transporting, giving rise to vanishingly small currents observed. It has been seen that the differential conductance and the thermal conductivity have qualitatively similar dependences on the bias voltage and temperature, while the thermopower and the Peltier coefficient share similar behaviors with bias voltage as well as temperature. The Wiedemann-Franz law was found to be violated, and the inelastic tunneling spectroscopy was observed to be temperature independent. Some of our observations are found to be qualitatively consistent with experiments. The physical reasonings concerning these features were also discussed. Since the measurements on the thermoelectric properties of spin-valve systems are scarce, we expect that the features we observed in this paper would be detected experimentally in near future.

Finally, we would like to point out that although the preceding observation was obtained on the basis of a tight-binding model, and the electron-electron interactions enter into the system only through the characteristic potential, our framework might be suitable for more complicated models. The only problem for a complicated model is to find a reliable way to get Green's function. A generalization of our treatment to include the effect of external fields is straightforward, which can be used to study the JMR ratio of the spin-valve system. Furthermore, we should mention that in our model we have neglected the effects of disorders, spin-wave scatterings, band structures, Coulomb blockade, and so forth on transport properties, and have assumed spin conservation during tunneling. These factors are also crucial to the spin-polarized tunneling. On the other hand, our obtained results on the differential conductance as well as the IET spectroscopy are still not able to be used to directly quantitatively compare with the existing experimental findings,[15] where the effect of magnon scatterings were emphasized. How to develop a theory including the above-mentioned factors to fit into experiments on a spin-valve system within Büttiker's gauge invariance and charge conserving transport framework, is still an open question, which is now in progress.

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*Corresponding author. Email address: gsu@cc6.gsbustc.ac.cn

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