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Plasmonic Thermal Conductance of Stack of Metallic Nanorings

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Abstract

In this paper, we study the plasmonic thermal conductance of ordered stacks of metallic nanorings in a host material. Using second quantized formalism of the Random Phase Approximation, we first determine the dispersion relations of surface plasmon waves on the stacks of nanorings. Then, using Landauer-Buttiker formalism, we determine the coefficient of plasmonic thermal conductance and heat current through the stack as a function of temperature, radius, spacing of rings and dielectric constant of host material. Our results indicate that ordered stacks of metallic nanorings have potential plasmonic thermal properties for heat transfer in nanostructures.

Keywords: Nanostructures; Collective phenomena; Plasmons; Quantum ring; Heat transport

Introduction

Understanding the heat transfer between two objects that are nanometric apart is an important problem in nanostructures [1-5]. The possibility of heat transfer in ordered array of metallic nanoparticles has recently been an active area of research. One class of such structure which has been studied thoroughly, is a linear chain of non contacting spherical metallic nanoparticles [6, 7]. For a chain of metallic nanospheres, when the separation distance between them decreases, the oscillating moments due to plasmon excitations on the individual spheres couple together via Coulomb interaction. The coupling of the oscillating moments of the nonospheres results into propagating Surface plasmon (SP) modes with definite dispersion relation. The frequencies of these SP modes depend on the size and the charge density of nanoparticles [8-13].

Heat can be transported along such a chain by surface plasmon wave excited thermally at one end of chain. The heat transfer properties of such structure which depend on the dispersion relations of the propagating SP modes are fixed once the size, the charge density, the relative distance between the nanoparticles and the dielectric constant of the surrounding material are set.

In this paper, we consider plasmonic thermal conductance of a chain of ordered metallic nanorings for transport of heat in nanostructures. For an ideal zero thickness nanoring the excited plasmon waves have discrete frequencies [14]. These plasmon waves cause the electron charge density in the nanoring to oscillate. The field produced by the oscillating charge density, in the non-retarded limit, couples neighboring rings through their Coulomb interaction which results in propagating SP modes. Such a chain can be used to transfer thermal energy between nanostructures by thermally exciting SP modes at one end of chain.

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The organization of the paper is as follows: In section II, we present the second quantized Hamiltonian for zero thickness nanoring and describe the formalism needed to calculate the plasmon frequencies for finite and infinite ordered stacks of nanorings. In section III, we will describe the Landauer-Buttiker formalism for calculating the plasmonic thermal conductance of the chain of the metallic nanorings. Finally, the numerical results for dispersion relations of surface plasmon waves, the plasmonic thermal conductance of such stack and conclusions are presented in section IV.

Materials and Methods

I. Formalism

We model the nanoring with zero thickness one dimensional circular shape jellium with radius R, consisting of conducting electrons, confined to the ring, and a uniformly distributed positive background charges. We assume that the ring is embedded in a dielectric medium with dielectric constant ε_s and the interactions between the electrons is the normal Coulomb interaction, $e^2/\varepsilon_s r$, down to the classical radius of electron.

Considering the xy-plane as the plane of ring, following ref [14], the Hamiltonian of the single ring in terms of annihilation and creation operators, $a_{n\alpha}$, $a^{\dagger}_{n\alpha}$, of single particle kinetic energy eigenstates has the form

$$\widehat{H} = \sum_{n,\alpha} \varepsilon_n a^{\dagger}_{n\alpha} a_{n\alpha} + \frac{1}{4\pi R} \sum_{\substack{m,n,n' \\ m\neq 0}} \sum_{\alpha,\alpha'} V(m)\, a^{\dagger}_{n+m,\alpha} a^{\dagger}_{n'-m,\alpha'} a_{n'\alpha'} a_{n\alpha}, \tag{1}$$

where

$$\varepsilon_n = \frac{\hbar^2 n^2}{2m^* R^2}, \tag{2}$$

and $V(m)$ is the mth component of the electron-electron interaction potential given By

$$V(m) = \frac{2e^2}{\varepsilon_s} Q_{|m|-\frac{1}{2}} (1 + 2(\frac{r_c}{R})^2). \tag{3}$$

In the above equations $Q_\nu(x)$ is the second kind Legendre function [15], m^* is the effective mass of electron, r_c is the classical radius of electron, $n = 0, \pm 1, \pm 2, \cdots$ is the angular quantum number, and $\alpha = 1, 2$ is the spin quantum number.

The plasmons frequencies can be determined from the zero's of the dielectric function of the nanoring. We use the Random Phase Approximation (RPA) form of the dielectric function which can be expressed in terms of free electron polarizability and the electron-electron interaction potential.

The field operators in the interaction representation for the electrons in the ring in terms of the single-particle eigenfunctions of their kinetic energy operator have the forms

$$\widehat{\psi}_{I\alpha}(\theta,t) = \frac{1}{\sqrt{L}} \sum_{n=-\infty}^{+\infty} a_{n\alpha} e^{-i\omega_n t} e^{in\theta} \eta_\alpha, \tag{4}$$

and

$$\widehat{\psi}^{\dagger}_{I\alpha}(\theta,t) = \frac{1}{\sqrt{L}} \sum_{n=-\infty}^{+\infty} a^{\dagger}_{n\alpha} e^{-i\omega_n t} e^{-in\theta} \eta^{\dagger}_\alpha, \tag{5}$$

where $\omega_n = \frac{\varepsilon_n}{\hbar}$, $L = 2\pi R$, and R is the radius of the ring. The free electron polarizability is defined by

$$\hbar \Pi^0(\theta t, \theta' t') = -i\, G^0_{\alpha\beta}(\theta t, \theta' t')\, G^0_{\beta\alpha}(\theta' t', \theta t), \tag{6}$$

where the repeated indices must be summed and $G^0_{\alpha\beta}(\theta t, \theta' t')$ is the non-interacting single particle Green function, defined in terms of the field operators by [16]

$$i\, G^0_{\alpha\beta}(\theta t, \theta' t') = \langle \Phi_0 | T\, [\widehat{\psi}_{I\alpha}(\theta,t) \widehat{\psi}^{\dagger}_{I\beta}(\theta',t')] | \Phi_0 \rangle \tag{7}$$

In the above equation, $|\Phi_0\rangle$ is the non-interacting ground state of the electrons. In terms of bases space of kinetic energy operators (KEB) the RPA dielectric function has the simple form

$$\varepsilon(n,\omega) = 1 - V(n)\, \Pi^0(n,\omega), \quad n = 0, \pm 1, \pm 2, \cdots \tag{8}$$

where ω is the angular frequency, $\Pi^0(n,\omega)$ and $V(n)$ are, respectively, the free-electron polarizability and the electron-electron interaction potential in (KEB).

Substituting eqs. (4) and (5) into eq. (7) and evaluating the ground state expectation value, we obtain the expression

$$G^0_{\alpha\beta}(n,\omega) = \delta_{\alpha\beta} [\frac{\Theta(|k_n| - |k_F|)}{\omega - \omega_n + i\eta} + \frac{\Theta(|k_F| - |k_n|)}{\omega - \omega_n - i\eta}], \tag{9}$$

for the single-particle Green function in (KEB). In the above equation Θ is the usual unit step function, $k_n = \frac{2\pi n}{L}$ is the wave number associated with the angular quantum number n, and $k_F = \frac{2\pi}{L}(n_F + \frac{1}{2})$ is the Fermi wave number with the Fermi angular quantum number n_F .

Finally, the free electron polarizability, $\Pi^0(n,\omega)$, can be obtained from the relation

$$\Pi^0(n,\omega)= -\frac{i}{\hbar}\frac{1}{\pi R}\sum_{n'=-\infty}^{+\infty}\int_{-\infty}^{+\infty}\frac{d\omega'}{2\pi}\,G^0(n',\omega')\,G^0(n'+n,\omega'+\omega) \quad (10)$$

where upon carrying the frequency integral, we obtain

$$\Pi^0(n,\omega)= \frac{1}{\pi\hbar R}\sum_{m=-\infty}^{+\infty}\Big[\frac{\Theta(|k_F|-|k_m|)\Theta(|k_{m+n}|-|k_F|)}{\omega-[\omega_{m+n}-\omega_m]+i\eta} -\frac{\Theta(|k_F|-|k_m|)\Theta(|k_{m-n}|-|k_F|)}{\omega+[\omega_{m+n}-\omega_m]-i\eta}\Big]. \quad (11)$$

Substituting the above relation in eq. (8) and setting the resulting equation equal to zero the various plasmon modes of nanoring can be determined.

II. Finite and Infinite Length Stacks of Nanorings

In this section, we consider both finite and infinite length stacks of ordered array of identical nanorings with radius, R, and spacing, a. We assume that the stack is imbedded in a dielectric medium with dielectric constant, ε_s . Taking the axes of the stack in the z-direction, the Hamiltonian of the system is sum of the Hamiltonians of the individual rings, given by eq. (1), and a part, $\hat{V}$, describing the total Coulomb interaction energies between the rings. This last part causes the transfer of electromagnetic energy between the rings along the stack and is given by

$$\hat{V}=\frac{1}{2}\sum_{i\neq j}\int d\theta_i\int d\theta_j\;\rho(\theta_i)\,V(\theta_i-\theta_j)\,\rho(\theta_j), \quad (12)$$

where $\rho(\theta_i)$ is the electron density operator of the ith ring, and

$$V(\theta_i-\theta_j)=\frac{e^2}{2\varepsilon_s R}\Big[\sin^2\Big(\frac{\theta_i-\theta_j}{2}\Big)+\Big(\frac{a|i-j|}{R}\Big)^2\Big]^{-\frac{1}{2}}, \quad (13)$$

is the Coulomb interaction potential between the ith and jth rings, where a is the distance between nearest two rings.

Using the RPA polarizability function of the individual rings and the linear response function the dispersion relations of the SP plasmon waves can be determined within the RPA. In the (KEB) the induced electron density on the ith ring due to induced fields of other rings, is given by

$$\delta\rho_i(n,\omega)=\kappa_i(n,\omega)\sum_{i\neq j}V_{i,j}(n)\;\delta\rho_j(n,\omega),$$
$$n=0,\pm1,\pm2,\cdots \quad (14)$$

where $\kappa_i(n,\omega)=\dfrac{\Pi^0(n,\omega)}{1-V_{i,i}\,\Pi^0(n,\omega)}$ is the RPA polarizability of the ith ring and $V_{i,j}(n)$ is the Coulomb interaction potential between the ith and the jth rings, given by

$$V_{i,j}(n)=\frac{2e^2}{\varepsilon_s}Q_{|n|-\frac{1}{2}}\Big(1+2\Big(\frac{a|i-j|}{R}\Big)^2\Big). \quad (15)$$

If we consider only nearest neighbor interactions for ordered array of identical nanorings, eq. (14) reduces to

$$\delta\rho_i(n,\omega)=\Pi_i^0(n,\omega)\,[V_{i,i}\;\;\delta\rho_i(n,\omega) +V_{i,i+1}\,\delta\rho_{i+1}(n,\omega)+V_{i,i-1}\,\delta\rho_{i-1}(n,\omega)],$$
$$i=0,\pm1,\pm2,\cdots \quad (16)$$

where

$$V_{i,i+1}(n)=V_{i,i-1}(n)=V_{12}(n)\quad i=0,\pm1,\pm2,\cdots \quad (17)$$

and

$$V_{i,i}(n)=V_{11}(n)\quad i=0,\pm1,\pm2,\cdots \quad (18)$$

Fourier transforming eq. (16), we obtain

$$\{1-\Pi^0(n,\omega)\,[V_{11}(n) + 2V_{12}(n)\cos(ak)]\}\,\delta\rho(k,n,\omega)=0 \quad (19)$$

where for infinite number of rings, the range of k is $[\frac{-\pi}{a},\frac{\pi}{a}]$ and

$$\delta\rho(k,n,\omega)=\sqrt{\frac{a}{2\pi}}\sum_{l=-\infty}^{+\infty}\rho_l(n,\omega)\,e^{-ialk}. \quad (20)$$

For finite number of rings, say N , if we take the origin of the z-axis at one end of the stack, with open bounding condition, the possible values for k are $k_n=\dfrac{2n\pi}{(N+1)a}$, with $n=1,2,\cdots,N$.

Finally, setting the expression in the curly bracket of eq. (19) equal to zero, we obtain the dispersion relations for self-sustained SP waves on the stack of nanorings with finite or infinite number of rings.

III. Plasmonic Thermal Conductance of Stack of the Nanorings

Let us consider a chain of infinite length of nanorings in the host dielectric along the z-axis as shown in Figure 1. For determining the thermal conductance of this chain, we assume that the left part of the chain, $z < 0$, is maintained at temperature T and the section $z > L$ is kept at temperature $T + \delta T$. We also suppose that the temperature difference δT is small enough in comparison with the mean temperature $(2T + \delta T)/2$.

The thermally excited collective modes of electrons in nanorings transport thermal energy along the chain via the surface plasmon modes. In the linear regime, where there is no interaction between the SP modes, the transmission coefficients of SP modes from left to right and vice versa are independent of frequency and are equal to one. For calculating the thermal current along the chain, we use the Landauer-Buttiker theory. According to the Landauer-Buttiker formalism, the energy current carried by the right and left moving surface plasmons are given by

$$\varphi^{+} = \frac{1}{2\pi} \sum_{\substack{m=-\infty \\ m\neq 0}}^{+\infty} \int_{0}^{\frac{\pi}{d}} \left| v^{+}_{gm}(k) \right| \hbar\omega_m(k) f^{+}_{B}[\omega_m(k)] dk, \qquad (21)$$

and

$$\varphi^{-} = \frac{1}{2\pi} \sum_{\substack{m=-\infty \\ m\neq 0}}^{+\infty} \int_{0}^{\frac{\pi}{d}} \left| v^{-}_{gm}(k) \right| \hbar\omega_m(k) f^{-}_{B}[\omega_m(k)] dk, \qquad (22)$$

where $\varphi^{\pm}$ are the energy currents, k is the wave vector, $\omega_m(k)$ is the dispersion relation of mth SP mode, $v_{gm}(k) = \frac{d\,\omega_m(k)}{dk}$ is the group velocity, and $f^{\pm}_{B}(\omega) = [\exp(\beta_{\pm}\hbar\omega) - 1]^{-1}$ is the Bose-Einstein distribution function. The thermal conductance of a stack due to heat transfer by SP modes is given by

$$G = \lim_{\delta T \to 0} \frac{\varphi^{+}(T + \delta T) - \varphi^{-}(T)}{\delta T}. \qquad (23)$$

Using eqs (21) and (22), in the limit of $\delta T \to 0$ we obtain the expression

$$G = \frac{\hbar^2}{2\pi k_B T^2} \sum_{m} \int_{0}^{\frac{\pi}{d}} \omega^2_m(k) \left| v_{gm}(k) \right| \frac{e^{\beta\hbar\omega_m}}{(e^{\beta\hbar\omega_m} - 1)^2} dk, \qquad (24)$$

for the coefficient of thermal conductance.

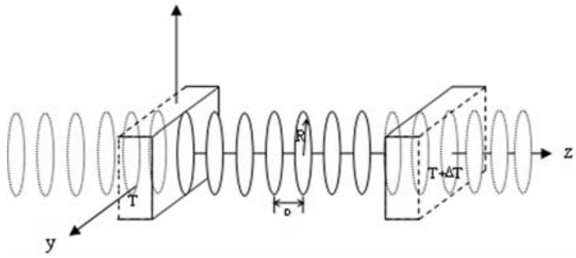

Figure 1. A chain of infinite length of nanorings in the host dielectric along the z axis, with spacing D and radius R.

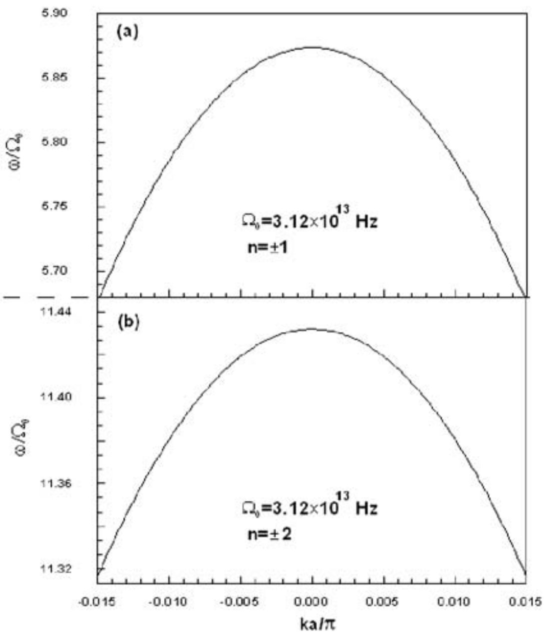

Figure 2. The behavior of plasmon frequencies of infinite stack of ordered nanorings imbedded in dielectric medium with dielectric constant equal to 14 for orbital quantum numbers ±1 and ±2 as a function of wave vector.

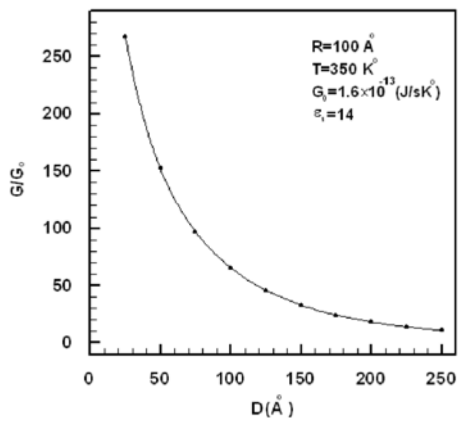

Figure 3. The plasmonic coefficient of thermal conductance of the stack as a function of ring spacing.

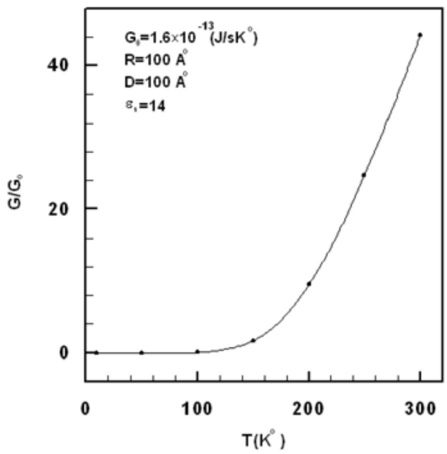

Figure 4. The plasmonic thermal conductance of an stack of metallic nanorings with radius, R = 100 Å, spacing D = 100 Å, and dielectric constant ε_s = 14 as a function of temperature.

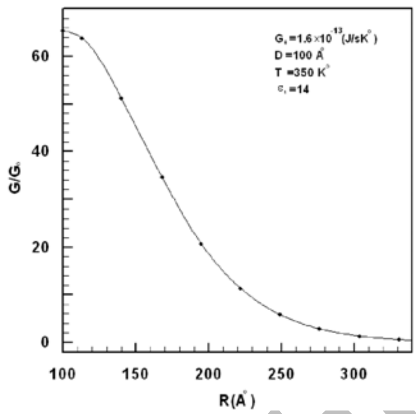

Figure 5. The plasmonic thermal conductance of an stack of metallic nanorings with spacing D = 100 Å, and dielectric constant ε_s = 14, in T=350 K° as a function of radius of nanorings.

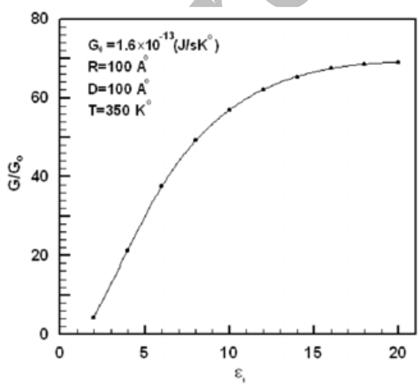

Figure 6. The plasmonic thermal conductance of an stack of metallic nanorings with spacing D = 100 Å, and radius R = 100 Å in T = 350 K° as a function of dielectric constant of host material.

Results and Discussion

For an stack of metallic nanorings with radius, R = 100 Å and spacing D = 100 Å we chose the number of electrons in each rings equal to 294. This gives us 2.02 for the dimensionless density parameter, r_s, which represents~Al. In the system of units in which $\hbar$ = 1 and $2m^*$ = 1, where m^* is the effective mass of the electron, the calculated SP dispersion relations for infinite stack of ordered nanorings imbedded in a dielectric medium with dielectric constant equal to 14 for orbital quantum numbers ±1 and ±2 are depicted in Figure 2.

The dependence of plasmonic coefficient of thermal conductance of the stack on its spacing is depicted in Figure 3. Figure. 4. represents the variation of the plasmonic thermal conductance as a function of temperature. We have also considered the effect of rings radius and the dielectric constant of host material on the thermal conductance. The results are presented in Figures. 5, and 6, respectively. Finally, the amount of heat current that can be transported via SP modes by the stack as a function of temperature difference with one side of the stack kept at fixed temperature of 350 K° is presented in Figure 7. The results indicates that an amount of 10^{-10}(J/s) of heat can be transferred per second by the stack.

In conclusion, we have shown that an ordered stack of metallic nanorings which supports propagating surface plasmon modes can be used for transfer of thermal energy. For metallic nanoring with R = 100 Å and spacing D = 100 Å and r_s = 2.02 in a medium with dielectric constant ε_s = 14 at temperature of 350 K°, the amount of heat current that can be transferred by SP modes is of order of 10^{-10}(J/s), thus, the stack of nanorings can also be used as a nano-heat sink in nanocircuits.

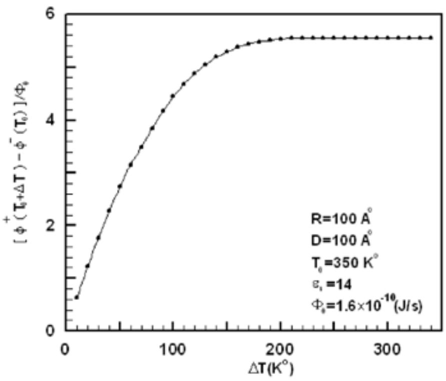

Figure 7. The variation of heat current transported by the SP modes of the stack as a function of temperature difference where one side of the stack is kept at fixed temperature of 350 K°.

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