COULOMB CORRELATION EFFECTS
ON THE HIGH FREQUENCY HOPPING
CONDUCTION IN DISORDERED SYSTEMS

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Recently, there has a renewed interest in studying the hopping conduction (HC). The new phenomena observed in various materials and the correspondingly theoretical descriptions are reported

(i) on the resistance crossovers induced by different factors (temperature [1], magnetic [2], and electric field [3]),

(ii) on negative magnetoresitances of different sources in both the nearest-neighbor hopping [4] and the variable-range hopping (VRH) [5], and

(iii) on the non-linear hopping conduction effects assumed to have an important impact on the performance of VRH thermometric sensors [6].

All these progresses, however, are associated with the *dc* hopping conduction, while there has a little of advancement in understanding the *ac* hopping conduction during last decades, though experimental data is continuously accumulated [7].

The fact that in the *ac* HC the electron transfer occurs only within a pair of localized states should be considered as the starting point in finding available theoretical approximations, which certainly differ from those used in calculating the *dc* HC. In the so-called relaxation regime of the high frequency HC the electron transfer between states is assisted by phonons. Following the pair approximation suggested originally by Pollak and Geballe [8] the main contribution to the high frequency HC is given by the pairs with the transition frequency of the order of the external electrical field frequency ω. The separation between states in such the pairs could be estimated by:

$$r_\omega = \frac{\xi}{2} \ln \frac{\nu_{ph}}{\omega},$$

(1)

where ξ is the localization length, ν_{ph} is a characteristic frequency of the order of the phonon frequency ($\approx 10^{12} \div 10^{13} s^{-1}$). The procedure of calculating the conductivity $\sigma(\omega)$ consists of two steps: to calculate the conductivity for a single pair and to average this conductivity over all the possible pairs. The most important feature of pairs regarded in the approximation [8] is that for each pair the electron hopping rate between sites inside pair is much greater than that between an inside site and an outside one. In other words, each pair should be seen as a closed subsystem with the induced dipole moment [9]:

$$q_d(\omega, \Omega, r) = er(e\mathbf{E}r/k_B T)[4\cosh^2(\Omega/2k_B T)]^{-1}(1 + i\omega\tau)^{-1}.$$

(2)

where $\mathbf{E}$ is the electrical field with the frequency ω, $\mathbf{r}$ is the d-dimensional vector connecting two sites of the pair, e is the elementary charge, and ω is the activation energy (i.e. the energy necessary for transferring an electron between sites in the pair). The transfer is suggested due to phonon assisted tunneling with characteristic frequency:

$$\tau^{-1} = \nu_{ph} \exp(-2r/\xi).$$

(3)

The dipole moment per unit volume (area) could then be defined as

$$Q_d(\omega) = \iint q_d(\omega, \Omega, T) \mathcal{F}_d(\Omega, r, T) d\Omega d\mathbf{r}. \tag{4}$$

here $\mathcal{F}_d(\Omega, r, T)$ is the distribution function of pairs in the sence that the quantity $2(d - 1)\pi \mathcal{F}_d(\Omega, r, T) r^{d-1} d\mathbf{r}$ gives the probability of finding in a unit volume (area) a pair of an empty and an occupied site with a separation $\in [\mathbf{r}, \mathbf{r} + d\mathbf{r}]$ and with an activation energy $[\Omega, \Omega + d\Omega]$.

The relaxation losses are defined as [9]:

$$\sigma_d(\omega) = -\mathrm{Im} Q_d(\omega) \omega / E. \tag{5}$$

ubstituting eqs. (2) - (4) into eq. (5) we have:

$$\sigma_3(\omega) = \frac{\pi}{96} e^2 \xi^5 \omega^2 \int_{1/\nu_{ph}}^{\infty} \ln(\nu_{ph}\tau)^4 \frac{d\tau}{1 + \omega^2\tau^2} \int_0^{\infty} \frac{\mathcal{F}_3(\Omega, r_\tau, T)}{k_B T \cosh^2(\Omega/2k_B T)} d\Omega. \tag{6}$$

$$\sigma_2(\omega) = \frac{\pi}{64} e^2 \xi^4 \omega^2 \int_{1/\nu_{ph}}^{\infty} \ln(\nu_{ph}\tau)^3 \frac{d\tau}{1 + \omega^2\tau^2} \int_0^{\infty} \frac{\mathcal{F}_2(\Omega, r_\tau, T)}{k_B T \cosh^2(\Omega/2k_B T)} d\Omega. \tag{7}$$

Since the main contribution to integrals in eqs. (6), (7) are given by the pairs of $\approx \omega^{-1}$, to the first approximation we have:

$$\sigma_3(\omega) = \frac{\pi^2}{192} e^2 \xi^5 \omega \ln\left(\frac{\nu_{ph}}{\omega}\right)^4 \int_0^{\infty} \frac{\mathcal{F}_3(\Omega, r_\omega, T)}{k_B T \cosh^2(\Omega/2k_B T)} d\Omega. \tag{8}$$

$$\sigma_2(\omega) = \frac{\pi^2}{128} e^2 \xi^4 \omega \ln\left(\frac{\nu_{ph}}{\omega}\right)^3 \int_0^{\infty} \frac{\mathcal{F}_2(\Omega, r_\omega, T)}{k_B T \cosh^2(\Omega/2k_B T)} d\Omega. \tag{9}$$

The distribution function of pairs is defined as [9]:

$$\mathcal{F}_d(\Omega, r, T) = \int_0^{\infty} g(\epsilon_1) d\epsilon_1 \int_{-\infty}^{0} g(\epsilon_2) d\epsilon_2 \delta\left(\epsilon_1 - \epsilon_2 - \frac{e^2}{\kappa r} - \Omega\right). \tag{10}$$

ere, κ is the dielectric constant, $g(\epsilon)$ is the density of states (DOS) near the Fermi level. he single electron energy ϵ_i is measured from the Fermi level. The term $e^2/\kappa r$ in the rgument of the δ-function in eq. (10) describes the Coulomb electron-electron correlation.

Following the expression of eq. (10) the function $\mathcal{F}_d(\Omega, r, T)$ is essentially determined by the form of the DOS. Neglecting electron-electron interaction, Mott [10] suggested $g(\epsilon) \equiv G_0 = $ const. which leads to the famous $T^{-1/(d+1)}$-law for dc conductivity. fros-Shklovskii (ES) [11] have shown that, as a consequence of the Coulomb correlation etween localized states, the DOS tends to zero near the Fermi level, giving rise to the oulomb gap:

$$g_d(E) = \alpha_d |E|^{d-1}, \alpha_d = (d/\pi)(\kappa/e^2)^d \tag{11}$$

nd further to the $T^{-1/2}$-law for temperature dependence of dc-conductivity. To describe crossover from Mott-$T^{-1/(d+1)}$-law to ES-$T^{-1/2}$ law, Nguyen [12, 13] suggested for DOS general form:

$$g_d(E) = \alpha_d E_d^{d-1} \frac{|E|^{d-1}}{E_d^{d-1} + |E|^{d-1}}. \tag{12}$$

where E_d is an adjustable parameter. The DOS of eq. (12) tends to the Mott constant DOS in the limit of $|E| >> E_d$ and to the Coulomb gap DOS of eq. (11) in the opposite limit. Recently [14], using the DOS of eq. (12), we obtained general expressions for describing the VRH thermos power crossover from the Mott $T^{(d-1)/(d+1)}$-behavior of constant DOS to the temperature-independent behavior of Coulomb gap.

Concerning the *ac* HC, Austin and Mott used the constant DOS $g(\epsilon) = G_0$ to calculate the conductivity σ_3 for 3D systems at finite temperature and found the law $\sigma_3(T) \propto T$ [10]. Using the same method, but with the DOS of eq. (11), ES [9,15] obtained expressions for $\sigma_3(\omega)$ in the high and low frequency limits at zero temperature. In the present work, by using the general DOS of eq. (12) the *ac* conductivity will be calculated in a large ranges of frequency and temperature for both 2D and 3D cases. The obtained expressions include Austin-Mott and ES results as the limited cases. The calculating procedure is standard as mentioned above and will be shortly shown below.

Substituting eq. (12) into eq. (10) we find the distribution functions of pairs respectively, for 2D and 3D systems:

$$\mathcal{F}_3(\Omega, r, T) = \alpha_3^2 E_3^5 \left[Z - 2\mathrm{arctg}(Z) + 2\frac{\mathrm{arctg}(Z)}{Z^2 + 4} + 2\frac{\ln(Z^2 + 1)}{Z(Z^2 + 4)} \right]. \tag{13}$$

$$\mathcal{F}_2(\Omega, r, T) = \alpha_2^2 E_2^3 \left[Z - 2\ln(Z + 1) + 2\frac{\ln(Z + 1)}{Z + 2} \right]. \tag{14}$$

where $Z = \frac{\Omega}{E_d} + \frac{e^2}{\kappa r E_d}$

Now, the relaxation losses can be calculated by substituting eqs. (13) and (14) into eqs. (8) and (9), respectively. For the 3D case it gives finally:

$$\sigma_3(\omega, T) = \frac{\pi^2}{48} \alpha_3^2 E_3^4 \xi^4 \frac{e^4 \omega}{\kappa} \ln^3\left(\frac{\nu_{ph}}{\omega}\right) \left\{ \frac{1}{2} - \frac{\mathrm{arctg}W}{W} + \frac{\mathrm{arctg}W}{W(W^2 + 4)} + \frac{\ln(1 + W^2)}{W^2(4 + W^2)} \right.$$
$$\left. + (\ln 2)T_1 + \sum_{n=1}^{\infty} \frac{1}{n!} T_1^n F_3^{(n)}(0) \int_0^\infty \frac{x^n dx}{\cosh^2(x)} \right\}, \tag{15}$$

where

$$F_3(x) = -\mathrm{arctg}(x + W) + \frac{\mathrm{arctg}(x + W)}{(x + W)^2 + 4} + \frac{\ln[1 + (x + W)^2]}{(x + W)[4 + (x + W)^2]},$$

and $F_3^{(n)}(0)$ is n-th order derivative of the function $F_3(x)$ at $x = 0$. For the 2D case we have:

$$\sigma_2(\omega, T) = \frac{\pi^2}{32} \alpha_2^2 E_2^2 \xi^3 \frac{e^4 \omega}{\kappa} \ln^2\left(\frac{\nu_{ph}}{\omega}\right)$$
$$\left\{ \frac{1}{2} - \frac{\ln(W + 1)}{W} + \frac{\ln(W + 1)}{W(W + 2)} + (\ln 2)T_1 + \sum_{n=1}^{\infty} (-1)^n T_1^n \right.$$
$$\left[\frac{1}{n(W + 1)^n} + \frac{\ln(W + 1)}{(W + 2)^{n+1}} - \sum_{i=1}^{n} \frac{1}{n + 1 - i} \frac{1}{(W + 1)^{n+1-i}(W + 2)^i} \right]$$
$$\left. \int_0^\infty \frac{x^n dx}{\cosh^2(x)} \right\}. \tag{16}$$

here $W = \frac{e^2}{\kappa r_\omega E_d}$ and $T_1 = \frac{2k_b T}{E_d}$.

The obtained results of eqs. (15), (16) are very general in describing both the frequency and temperature dependencies of *ac* conductivity in large ranges of these parameters.

Firstly, we discuss the frequency dependence. In the limit of low temperatures, $T << e^2/\kappa r_\omega$, setting $T = 0$ in eqs. (15) and (16) we have:

$$\sigma_3(\omega) = \frac{\pi^2}{3} e^2 \omega \xi r_\omega^3 \left[1 - \frac{2}{W} \text{arctg}(W) + 2\frac{\text{arctg}(W)}{W(W^2+1)} + 2\frac{\ln(W^2+1)}{W^2(W^2+1)} \right]. \quad (17)$$

$$\sigma_2(\omega) = \frac{\pi^2}{8} e^2 \omega \xi r_\omega^2 \left[1 - \frac{2}{W} \ln(W+1) + 2\frac{\ln(W+1)}{W(W+2)} \right]. \quad (18)$$

Interestingly, in the case of high frequency $W = \frac{e^2}{\kappa r_\omega E_d} >> 1$ i. e., $\frac{r_\omega}{\xi} = \frac{1}{2} \ln\left(\frac{\nu_{ph}}{\omega}\right) <<$, these eqs. (17) and (18) respectively tend to the well-known ES [9] and Efros [15] formulas:

$$\sigma_3(\omega) = \frac{\pi^2}{48} (\alpha_3 E_3^2)^2 \frac{\xi^4 e^4}{\kappa} \omega [\ln(\nu_{ph}/\omega)]^3 \quad (19)$$

$$\sigma_2(\omega) = \frac{\pi^2}{8} (\alpha_2 E_2)^2 \frac{\xi^3 e^4}{\kappa} \omega [\ln(\nu_{ph}/\omega)]^2 \quad (20)$$

In the opposite limit of low frequency, $W << 1$, eqs. (17) and (18) tend to respectively:

$$\sigma_3(\omega) = \frac{\pi^2}{90} \alpha_3^2 \frac{e^{12}}{\kappa^5} \frac{\omega}{\ln(\nu_{ph}/\omega)} = \frac{1}{10} \frac{\kappa \omega}{\ln(\nu_{ph}/\omega)}, \quad (21)$$

$$\sigma_2(\omega) = \frac{\pi^2}{48} \alpha_2^2 \frac{e^8}{\kappa^3} \xi \omega = \frac{1}{12} \kappa \omega \xi. \quad (22)$$

The expressions (21) and (22) exactly coincide with those obtained by ES [9] and Efros [15], using the DOS of eq. (11). Note that, in the expressions of eqs. (21), (22) there absent the parameter G_0 that implies the obtained results are universal, independent of the studied disordered system model. These expressions also clearly show an important role of the Coulomb electron-electron correlation at low temperature.

Experimentally, the frequency dependence of conductivity is often assumed to have the form: $\sigma \propto \omega^s$ with the exponent $s \leq 1$. Using one electron approximation with nonzero density of states at the Fermi level, Austin and Mott [10] obtained:

$$s = 1 - 4[\ln(\nu_{ph}/\omega)]^{-1}. \quad (23)$$

which does not agree satisfactorily with the experimental data. In particular the experimental exponent s often increases as temperature decreases [16] and is much closer to unity than that predicted by eq. (23). For example, Abkowitz at al. [17] reported that $s = 1$ for a-Si. A possible reason of this discrepancy may be due to a correlation in the spatial distribution of site [9].

For our results, from eqs. (17), (18) we have:

$$s_3 = 1 - 3[\ln(\nu_{ph}/\omega)]^{-1} + s_{c3} \quad (24)$$

$$s_2 = 1 - 2[\ln(\nu_{ph}/\omega)]^{-1} + s_{c2} \quad (25)$$

where both the quantities s_{c2} and s_{c3} (see Appendix) are positive. The frequency dependencies of s_2 and s_3 are shown in Fig. 1. We see that both s_2 and s_3 decrease with increasing ω. Importantly, as can be seen in fig. 1, the present values of s_d are larger than Mott's and ES values and closer to the experimental value $s = 1$ of ref. [17].
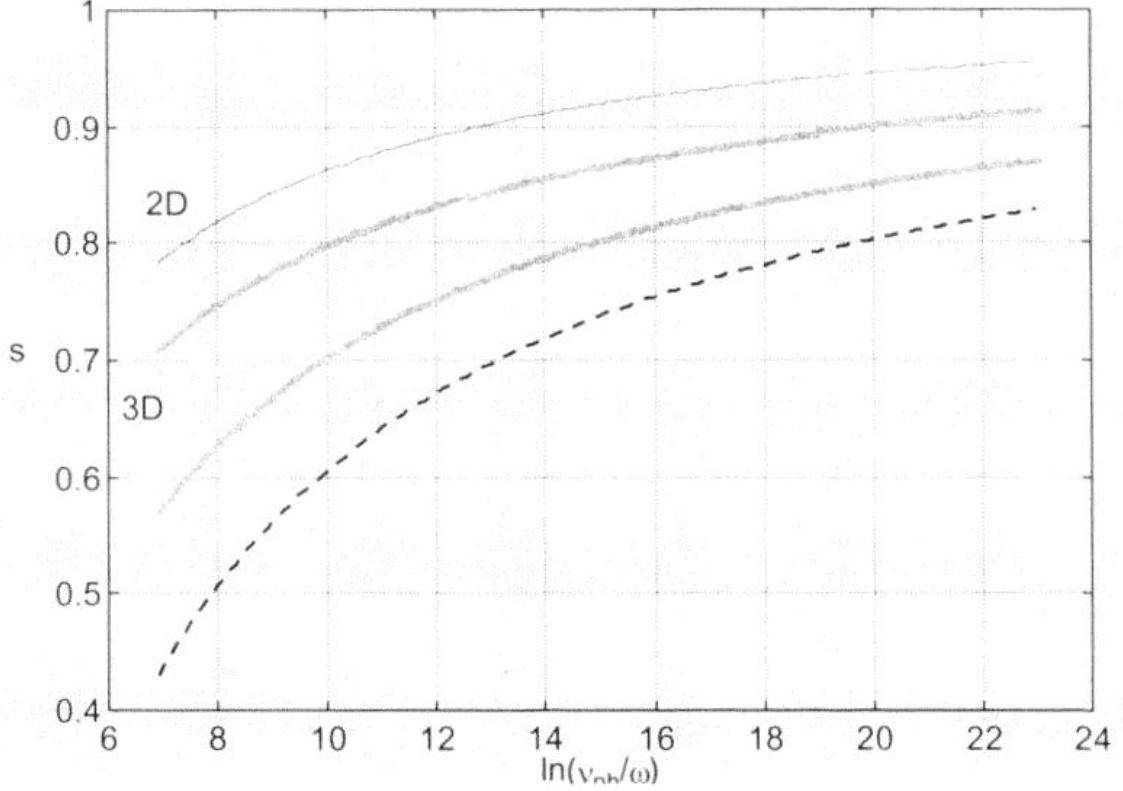

Fig. 1: The exponent $s = d(ln\sigma_d)/d(\ln \omega)$ is plotted against the $\ln(\nu_{ph}/\omega)$ follwing eqs. (23) and (24) with $\nu_{ph} = 10^{13}$ Hz.
* The frequency ranges from 10^3 Hz to 10^9 Hz.
* The fitting parameter: $A^* = 2e^2/(\kappa\xi E_d) = 60$ for both 2D and 3D cases.
* Full line - eqs. (24) and (25), dashed line - Austin-Mott eq. (23), dots - from ES-eqs. (19) and (20).

Let us now discuss the dependence of conductivity on temperature. Neglecting the Coulomb correlation term $e^2/\kappa r$ and using the constant DOS, Austin and Mott [10] obtained the 3D law:

$$\sigma_3^{AM}(\omega, T) = \frac{\pi^2}{48}\xi^5 e^2 \omega [\ln(\nu_{ph}/\omega)]^4 G_0^2 k_B T. \tag{26}$$

Using the same approximation, Efros [15] obtained the 2D law:

$$\sigma_2^{AM}(\omega, T) = \frac{\pi^2}{128}\xi^4 e^2 \omega [\ln(\nu_{ph}/\omega)]^3 G_0^2 k_B T. \tag{27}$$

For the present calculations, from eqs. (15) and (16), in zero approximation, we already have:

$$\sigma_3(\omega, T) = \frac{\pi^2}{3}(\ln 2)\alpha_3^2 E_3^4 e^2 \omega \xi^5 \ln^4\left(\frac{\omega_{ph}}{\omega}\right) k_B T. \tag{28}$$

$$\sigma_2(\omega, T) = \frac{\pi^2}{8}(\ln 2)\alpha_2^2 E_2^2 e^2 \omega \xi^4 \ln^3\left(\frac{\omega_{ph}}{\omega}\right) k_B T. \tag{29}$$

It is easy to show that, except numerical factors, these expression (22) and (29) are coincided with the Austin - Mott eq. (26) and Efros eq. (27), respectively. Thus, in the limit cases for both frequency and temperature dependencies our results tend exactly to the Mott-Austin or ES-expression, respectively.
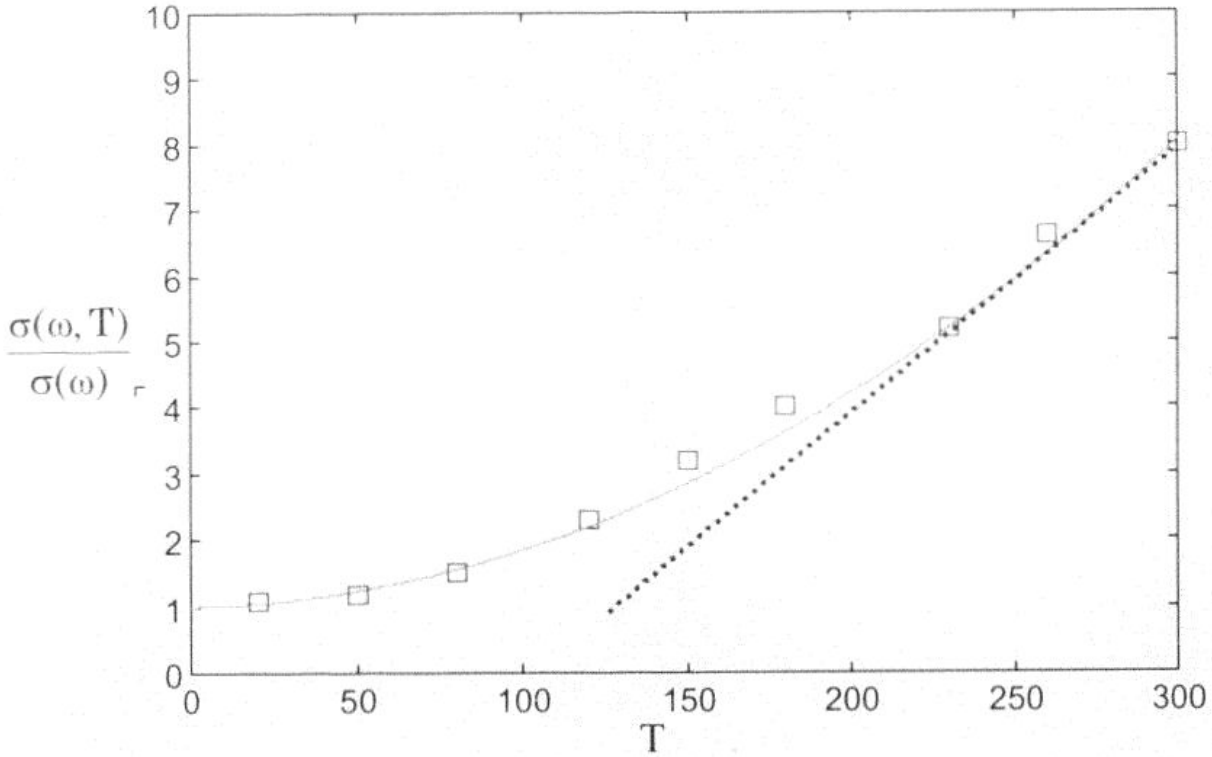

Fig. 2: Temperature dependence of the ac conductivity.
* Full line - eq. (29), dashed line - Austin-Mott eq. (26), squares - experimental points by Hauser et al. [19].

Concerning the temperature dependence, experimentally, at low temperature the temperature dependence of *ac* conductivity is much weaker than that resulted from eqs. (26, 27) [18]. Hauser at al. [19] reported that $\sigma_3(T)$ for a-Si saturates at low temperatures and the linear temperature dependence given by eq. (26) is not seen at temperature $T \approx 100K$. In order to describe such the $\sigma_3(T)$- behavior, we should keep the term proportional to T^2, in expressions (15) and (16). It is easy to show that the relaxation conductivity has then the form:

$$\sigma(\omega, T) = \sigma(\omega) + AT + BT^2, \tag{30}$$

where A and B are positive factors with $A >> B$. Using for a-Si values $\xi = 10A, \kappa = 10$ we obtain at $\omega = 10^4 s^{-1}$ that $A = 1, 1.10^{-3}$ and $B = 7, 5.10^{-5}$. In fig.2 we plot $\sigma(\omega, T)/\sigma(\omega)$ for an a-Si sample and compare experimental data [19] (squares) with the values calculated from Eqs. (30) (Full line) and (26) (dashed line). It is clear that the full line of the present work is in well agreement with the data of ref. [19] in large temperature range.

In conclusion, using the general form of DOS (12) we have obtained analytical expressions for describing the dependence of ac relaxation conductivity on frequency and temperature for both 2D and 3D cases. The obtained expressions tend to the well-known Mott and ES results in the limit of high and low frequencies. Concerning the temperature

dependence, including the term proportional to T^2, our result describes well experimental data for a-Si. The fact that in the theory there is only one parameter E_d gives an easy in making comparisons with experiments.

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Appendix: For exponent $s_d(d = 2$ or $3)$ from eqs. (17) and (18) we have:

$$s_d = \frac{d\ln\sigma}{d\ln\omega} = 1 - d[\ln(\nu_{ph}/\omega)]^{-1} + s_{cd}$$

where:

$$s_{c3} = \frac{2}{A^*}\frac{-\frac{2W}{W^2+4} + \mathrm{arctg}(W) - 3\frac{\mathrm{arctg}(W)}{W^2+4} + \frac{8\mathrm{arctg}(W)}{(W^2+4)^2} - 2\frac{\ln(W^2+1)}{W(W^2+4)} - 2\frac{W\ln(W^2+1)}{(W^2+4)^2}}{1 - 2\frac{\mathrm{arctg}(W)}{W} + 2\frac{\mathrm{arctg}(W)}{W(W^2+4)} + 2\frac{\ln(W^2+1)}{W^2(W^2+4)}}.$$

$$s_{c2} = \frac{2}{A^*}\frac{-\frac{W}{W+2} + \ln(W+1) - 2\frac{\ln(W+1)}{W+2} + 2\frac{\ln(W+1)}{(W+2)^2}}{1 - \frac{2}{W}\ln(W+1) + 2\frac{\ln(W+1)}{W(W+2)}}.$$

with $A^* = \frac{2e^2}{\kappa\xi E_d}$.

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ẢNH HƯỞNG CỦA TƯƠNG TÁC COULOMB LÊN DẪN NHẢY TẦN SỐ CAO TRONG CÁC HỆ KHÔNG TRẬT TỰ

Đặng Đình Tới

Khoa Vật Lý, Đại học Khoa học Tự nhiên- ĐHQG Hà Nội

Bằng cách sử dụng một hàm mật độ trạng thái tổng quát hơn đã nhận được biểu thức giải tích của độ dẫn điện xoay chiều phụ thuộc tần số và nhiệt độ trong dải rộng các giá trị tham số cho cả hệ hai và ba chiều. Trong các trường hợp giới hạn, các biểu thức này dẫn về các kết quả đã biết của các tác giả khác. Kết quả nhận được mô tả tốt số liệu thực nghiệm của a-Si.