

A variational study of electronic thermal conductivity of Anderson lattice model: an application to CMR manganites ($\text{Re}_{1-x}\text{A}_x\text{MnO}_3$)

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PACS 71.10.Fd, 75.47.Gk, 65.40.-b

ABSTRACT Using the variational method, we have investigated the temperature dependence of the electronic thermal conductivity (k_{el}) in rare-earth manganites doped with alkaline-earth ions, which display the well-known CMR behavior. The analysis is based on a two-band ($l-b$) Anderson lattice model Hamiltonian appropriate for the strong electron-lattice Jahn–Teller (JT) coupling regime, consistent with two-fluid descriptions incorporating ($l-b$) hybridization. Key model parameters includes Coulomb repulsion U , strong Hund's coupling J_H between e_g and t_{2g} spins and hybridization V between l -polarons and d -electrons of the same spin. In the ferromagnetic metallic phase, calculations show that the k_{el} increases with increasing temperature and near the transition temperature $T_c \approx 400$ K, it shows a minimum or a dip in k_{el} for a fixed value of V , J_H and x . The results of k_{el} exhibit a typical crystalline character with grain boundary scattering as a main mechanism limiting the heat transfer in these compounds.

KEYWORDS Anderson lattice model hamiltonian, CMR manganites, electronic thermal conductivity, variational method

FOR CITATION Rahul Saini, Sunil Panwar A variational study of electronic thermal conductivity of Anderson lattice model: an application to CMR manganites ($\text{Re}_{1-x}\text{A}_x\text{MnO}_3$). *Nanosystems: Phys. Chem. Math.*, 2026, **17** (3), 311–316.

1. Introduction

Manganites of perovskite structure, with the general formula $\text{Re}_{1-x}\text{A}_x\text{MnO}_3$ (where $\text{Re} = \text{La, Pr, Nd, etc.}$, and $\text{A} = \text{Ca, Sr, Ba, etc.}$) have gained tremendous significance across condensed matter research due to the strong coupling between their charge, orbital, and spin degrees of freedom [1,2]. These materials drew remarkable scientific attention following the discovery of colossal magnetoresistance (CMR), a striking phenomenon in which the resistivity drastically decreases upon application of a magnetic field [3,4]. The CMR effect, since its discovery, has motivated extensive theoretical and experimental studies owing to its relevance in magnetic sensing, data storage, and spintronic device applications.

Several theoretical frameworks have been proposed to explain the underlying mechanisms responsible for the celebrated CMR effect. The double exchange (DE) mechanism, arising from electron hopping between Mn^{3+} and Mn^{4+} ions, provides a fundamental understanding of ferromagnetism and metallic conduction in these oxides [5]. However, the DE model alone cannot account for all the transport and magnetic properties observed in doped manganites. Additional mechanisms such as the Jahn-Teller (JT) effect [6], polaronic interactions, and phase separation [7,8] have been introduced to explain the wide range of experimental results. The interplay between these effects gives rise to a wide variety of electrical and magnetic behaviours in doped manganites, revealing the profound role of lattice distortions and electron correlations in determining their macroscopic properties.

Among various thermal properties of doped CMR manganites, thermal conductivity (k) stands out as an important probe of the scattering processes of phonons and electrons, providing valuable insights into the complexity of charge-lattice interactions in these compounds. A careful examination of previous studies reveals two major thermal transport behaviours [9,10]. In the paramagnetic insulating phase, k is typically low and displays an amorphous-like temperature dependence ($dk/dT > 0$), suggesting dominant phonon scattering and localized electronic states. Conversely, in the ferromagnetic-metallic phase, k exhibits a crystalline-like behaviour ($dk/dT < 0$), indicative of coherent heat transport and delocalized charge carriers. The crossover between these two regimes occurs near the Curie temperature (T_c), producing a characteristic minimum in $k(T)$. This transition, accompanied by the restructuring of MnO_6 octahedra, reflects the fundamental coupling between structural and electronic degrees of freedom in these materials.

Studies on CMR materials have also employed many advanced many-body theoretical approaches, such as dynamical mean field theory developed by T.V. Ramakrishnan [11] and the current-carrier density collapse (CCDC) model [12].

These approaches have been successful in explaining the transport behaviour over the entire temperature range. In particular, the CCDC model attributes the electrical transport mechanism to a temperature-dependent collapse in carrier density, while the electrical resistivity is governed by changes in the relative volume fractions of the paramagnetic and ferromagnetic phases.

Ramakrishnan et al. [11] proposed a theoretical model describing the coexistence of localized Jahn–Teller (JT) polarons and itinerant band electrons in doped rare-earth manganites of the general form $\text{Re}_{1-x}\text{A}_x\text{MnO}_3$. According to their framework, this coexistence arises naturally under conditions of strong (JT) coupling and orbital degeneracy, offering a unified picture capable of accounting for the simultaneous presence of metallic conductivity and local distortions. Despite this theoretical progress, a quantitative explanation of electronic thermal conductivity (k_{el}) within a microscopic model that includes both hybridization and electron correlation remains lacking.

To address these limitations, Panwar et al. [13–16] introduced a variational approach based on the Anderson lattice model, initially developed to study the ground-state and thermal properties of heavy-fermion systems. This method was subsequently extended to examine magneto-transport phenomena, including thermoelectric power and electrical resistivity, in doped manganites across a wide temperature range and varying magnetic field conditions [17–19]. These studies demonstrated that the variational formalism successfully captures the temperature dependence of electrical resistivity $\rho(T)$ and the interplay between electronic correlations and spin disorder in such complex oxides. However, a detailed and systematic investigation of electronic thermal conductivity using this approach has not yet been undertaken.

In an ideal metallic system, the relationship between electronic and thermal conductivities is governed by the Wiedemann–Franz law [20], which predicts a constant Lorenz number under elastic scattering conditions. Nevertheless, for doped CMR manganites, this law often fails due to strong electron-phonon coupling, polaron formation, and spin fluctuations, which disrupt quasiparticle coherence [21, 22]. Therefore, a unified theoretical description capable of encompassing both electronic correlation and lattice distortion effects is essential for a complete understanding of thermal transport in these systems.

In this work, we present a variational study of electronic thermal conductivity (k_{el}) as a function of temperature for different doping concentrations x , hybridization strengths V , and Hund’s coupling J_H parameters in doped CMR manganites. This study extends the previously developed variational formalism, which had been successfully applied to model the temperature dependence of electrical resistivity $\rho(T)$ [17] and applies it to investigate thermal transport processes. The objective is to establish a microscopic framework that captures how hybridization and electron correlation collectively determine k_{el} and its deviation from conventional metallic behaviour.

2. Basic formulation

2.1. Model

In this study, a theoretical model is developed to quantitatively examine the electronic thermal conductivity (k_{el}) of doped colossal magnetoresistive (CMR) manganites within the strong electron-lattice Jahn–Teller (JT) coupling regime. We employ a Hamiltonian H_{lb} derived from the Anderson lattice formalism as proposed in earlier studies [11, 17], which effectively describes the coexistence of localized JT polarons (l -electrons) and itinerant band (b -electrons).

$$H_{lb} = - \sum_{\langle ij \rangle \sigma} \tilde{t}_{ij} (b_{i\sigma}^\dagger b_{j\sigma}) - \sum_{i\sigma} E_{jt} l_{i\sigma}^\dagger l_{i\sigma} + U \sum_{i\sigma} n_{i\sigma}^l n_{i\sigma}^b - J_H \sum_i \mathbf{s}_i \cdot \mathbf{S}_i - J_F \sum_{\langle ij \rangle} \mathbf{S}_i \cdot \mathbf{S}_j - \sum_{k\sigma} V_K (l_{k\sigma}^\dagger b_{k\sigma} + h.c.). \quad (1)$$

The details of symbols used are given in our previous work in Ref. [17].

Here, each term carries a specific physical significance. In Eq. (1), the b -electrons, which form a broad conduction band, hop between nearest-neighbor sites with an effective amplitude $\tilde{t}_{ij}$, while the localized l -polarons occupy energy levels at $-E_{JT}$ owing to the strong JT distortion. The term U represents the on-site Coulomb repulsion between l -polarons and b -electrons of identical spin at the same site i , while V_k is the l - b hybridization between l -polarons and b -electrons of the same spin. J_H is the Hund’s coupling that aligns the itinerant e_g spin ($\mathbf{s}_i$) with the localized t_{2g} core spin ($\mathbf{S}_i$), and J_F is the effective ferromagnetic exchange coupling between neighboring t_{2g} core spins ($\mathbf{S}_i, \mathbf{S}_j$). Together, these terms account for the essential competing interactions governing charge, spin, and lattice dynamics in CMR manganites.

In the case of finite U , the ground state of the system can be expressed by a modified variational wave function in k -space [17] as

$$\psi_{lb} = \prod_{k\sigma} [1 + A_{k\sigma} l_{k\sigma}^\dagger b_{k\sigma}] |\Phi_d\rangle, \quad (2)$$

where $|\Phi_d\rangle$ represents the Fermi Sea of delocalized d -electrons, and $A_{k\sigma}$ is the variational parameter characterizing the hybridization strength between localized and itinerant states. Optimization of the system’s energy expectation value with

respect to $A_{k\sigma}$ yields:

$$A_{k\sigma} = \frac{1}{2V_k} \left[\left(\epsilon_k + \frac{U}{2} n_\sigma^l - \epsilon_{d\sigma} \right) + \sqrt{\left(\epsilon_k + \frac{U}{2} n_\sigma^l - \epsilon_{d\sigma} \right)^2 + 4V_k^2} \right], \quad (3)$$

where

$$\epsilon_{d\sigma} = \frac{U}{2} n_\sigma^b + \frac{J_H}{2} n_\sigma^l - E_{JT} - J_F \sigma m - h. \quad (4)$$

Here, J_F involves the number of nearest neighbors and m is the site magnetization per atom given by

$$m = \frac{1}{N} \sum_{k\sigma} \sigma l_{k\sigma}^+ l_{k\sigma} \quad (5)$$

and N is the total number of lattice sites. The average occupation numbers for the itinerant b-electrons and localized l-electrons are defined as

$$n_\sigma^d = \frac{1}{N} \sum_k n_{k\sigma}^d, \quad n_\sigma^b = \frac{1}{N} \sum_k n_{k\sigma}^b = \frac{1}{N} \sum_k \frac{f_{k\sigma}^-}{(1 + A_{k\sigma}^2)} \quad (6)$$

and

$$n_\sigma^l = \frac{1}{N} \sum_k n_{k\sigma}^l = \frac{1}{N} \sum_k \frac{A_{k\sigma}^2 f_{k\sigma}^-}{(1 + A_{k\sigma}^2)}, \quad (7)$$

where $f_{k\sigma}^-$ is the Fermi–Dirac distribution function corresponding to the lower quasiparticle branch $E_{k\sigma}^-$

$$f_{k\sigma}^- = 1 / [\exp(\beta(E_{k\sigma}^- - \mu)) + 1] \quad (8)$$

with μ denoting the chemical potential and $\beta = 1/(k_B T)$. The lower quasiparticle energy branch, representing the hybridized electronic states, is then given by the following formula

$$E_{k\sigma}^- = \frac{1}{2} \left[\left(\epsilon_k + \frac{U}{2} n_\sigma^l + \epsilon_{d\sigma} \right) - \sqrt{\left(\epsilon_k + \frac{U}{2} n_\sigma^l - \epsilon_{d\sigma} \right)^2 + 4V_k^2} \right]. \quad (9)$$

This formulation allows the study of electronic structure renormalization arising from hybridization and correlation effects, offering a direct means of evaluating transport properties in manganites across different temperature and doping regimes.

2.2. Electrical resistivity

The electrical resistivity $\rho(T)$ serves as an essential precursor to determine the electronic component of thermal conductivity. Following the approach used in earlier variational studies [17], the temperature-dependent electrical conductivity $\sigma(T)$ is given by

$$\sigma(T) = \int \left(-\frac{\partial f_{k\sigma}^-}{\partial E_{k\sigma}^-} \right) \sigma'(E_{k\sigma}^-) dE_{k\sigma}^-, \quad (10)$$

where

$$\sigma'(E_{k\sigma}^-) = \sigma_0 [N^C(E_{k\sigma}^-)]^2 \quad (11)$$

and $N^C(E_{k\sigma}^-)$ represents the density of perturbed conduction band (e_g) states. This relation provides the link between the electronic structure and electrical transport, enabling the computation of resistivity as a function of temperature and hybridization parameters within the variational framework.

2.3. Thermal conductivity

In manganites exhibiting relatively high electrical resistivity, the contribution of electrons to the total thermal conductivity cannot be ignored, particularly in the ferromagnetic metallic phase. Here, the Wiedemann–Franz law [20] provides a phenomenological bridge between electrical and thermal transport. Neglecting lattice contributions, the electronic thermal conductivity k_{el} can be expressed as

$$k_{el} = \rho^{-1} L_0 T, \quad (12)$$

where $L_0 = 2.45 \times 10^{-8} \text{ W}\cdot\Omega/\text{K}^2$ is the Lorenz number, and ρ represents the electrical resistivity obtained from the variational calculations. Although deviations from the Wiedemann–Franz law have been observed experimentally in manganites due to strong electron-phonon coupling and localization effects, this relationship remains a reliable approximation in the ferromagnetic metallic region [21, 22]. The k_{el} calculations from resistivity data are plotted in Figs. 1–3.

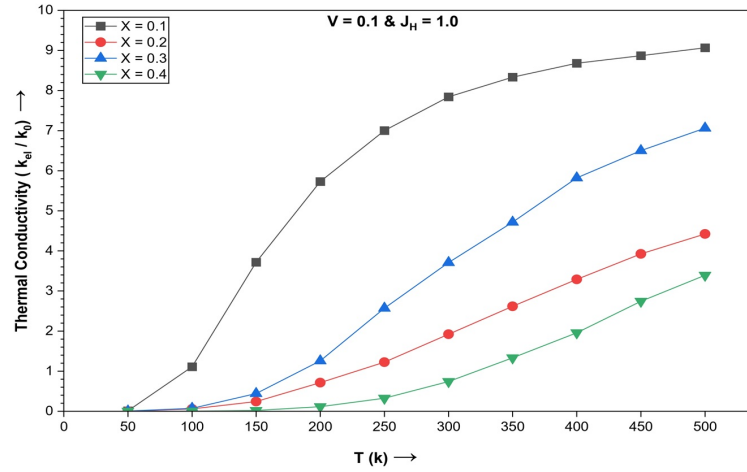


FIG. 1. Variation of electronic thermal conductivity k_{el} with temperature for different values of doping x at $V = 0.1$ and $J_H = 1.0$

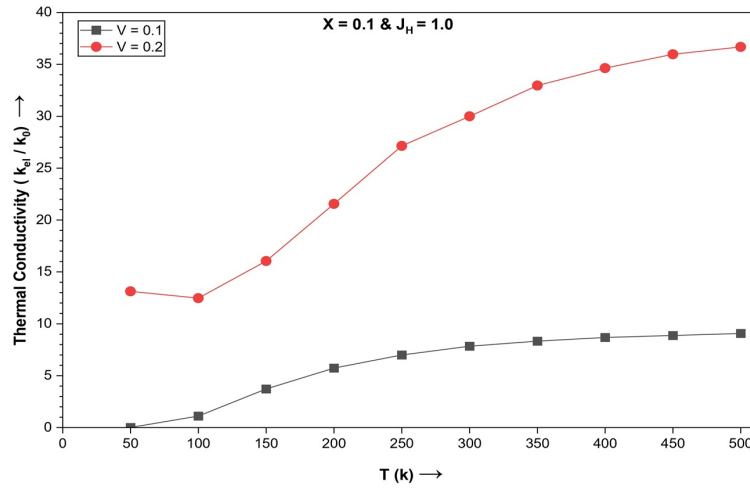


FIG. 2. Variation of electronic thermal conductivity k_{el} with temperature for different values of hybridization V at $x = 0.1$ and $J_H = 1.0$

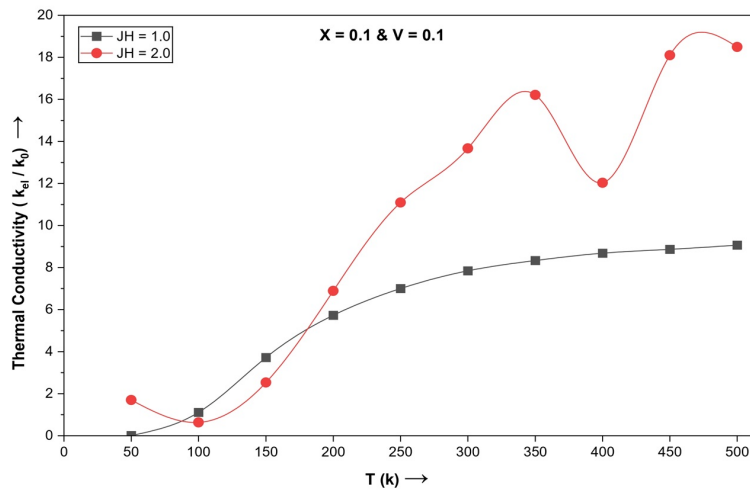


FIG. 3. Variation of electronic thermal conductivity k_{el} with temperature for different values of J_H at $x = 0.1$ and $V = 0.1$. Curve for $J_H = 2.0$ (red color) shows a minimum at transition temperature $T_c = 400$ K

3. Results and discussion

In the present calculations, the unperturbed conduction band of the three-dimensional manganite system is considered using a simple semi-circular density of states $N_{\sigma}^c(\epsilon_k) = (2/\pi)\sqrt{1 - \epsilon_k^2}$, centered around zero energy, which effectively captures the essential electronic structure of a strongly correlated perovskite lattice. The total bandwidth is taken as $W = 2.0$ eV, corresponding to realistic energy scales of e_g band electrons in CMR manganites. The on-site Coulomb interaction $U = 5.0$ eV, Jahn–Teller energy $E_{JT} = 0.5$ eV, hybridization strengths $V = 0.1$ and 0.2 eV and Hund’s coupling constants $J_H = 1.0$ and 2.0 eV. The Fermi energy $\epsilon_F = -0.238$ corresponds to a doping level of $x = 0.3$, while the doping concentration x itself is varied from 0.1 to 0.4 to investigate its effect on thermal transport.

In Figs. 1–3, we illustrate the temperature dependence of electronic thermal conductivity $k_{el}(T)$ for different values of doping (x), hybridization (V), and Hund’s coupling (J_H), respectively. Across all parameter sets, the general behavior of $k_{el}(T)$ exhibits a distinct crossover from low-temperature metallic characteristics to high-temperature insulating tendencies. In the ferromagnetic metallic region, we find that the $k_{el}(T)$ at low temperature increases with increasing temperature and near transition temperature $T_c \sim 400$ K it shows a minimum or a dip in k_{el} for a fixed value of hybridization V , Hund’s coupling J_H and doping x .

The behavior of k_{el} as a function of doping x is shown in Fig. 1. For a fixed hybridization strength V and Hund’s coupling (J_H), an increase in the doping concentration from $x = 0.1$ to 0.4 leads to a gradual decrease in $k_{el}(T)$ throughout the temperature range. Below $T = 150$ K, the thermal conductivity values for all doping levels are nearly identical, indicating that low-temperature transport is dominated by itinerant electron contributions with minimal influence from lattice distortions. However, at higher temperatures, the reduction in k_{el} becomes more pronounced for higher doping levels. This trend can be attributed to the increasing formation of Jahn–Teller polarons, which act as effective scattering centers for both charge carriers and phonons, thereby reducing the overall electronic contribution to thermal transport [9, 21]. The decrease in magnitude of k_{el} with increasing x , thus, signifies enhanced lattice disorder and polaronic scattering, consistent with experimental observations [4].

Figures 2 and 3 further illustrate the dependence of k_{el} on the hybridization parameter (V) and Hund’s coupling (J_H), respectively. A systematic increase in both parameters leads to a noticeable enhancement in k_{el} , accompanied again by a pronounced dip at $T_c \approx 400$ K. The increase in k_{el} with higher V indicates that greater hybridization strengthens the coupling between localized and itinerant states, thereby facilitating more coherent electronic transport and reducing localization effects. Similarly, a higher Hund’s coupling (J_H) enhances the alignment of the e_g electron spins with the localized t_{2g} core spins, promoting spin-polarized conduction and thus improving thermal transport efficiency in the ferromagnetic metallic phase [5].

For $J_H = 2.0$ eV, $V = 0.1$ eV and $x = 0.1$, a well-defined minimum in $k_{el}(T)$ is observed at $T_c = 400$ K beyond which thermal conductivity increases sharply with temperature (Fig. 3). This minimum corresponds to the transition region where spin disorder scattering and polaron formation reach their maximum influence. Above T_c , the increasing thermal agitation and breakdown of magnetic ordering lead to carrier localization, thereby reducing the electronic contribution to thermal conduction. Such behavior aligns with experimental trends reported for doped manganite samples such as $\text{Pr}_{0.6}\text{Sr}_{0.35}\text{Ag}_{0.05}\text{MnO}_3$ [22].

The overall results obtained from this variational formulation qualitatively reproduce the experimentally observed features of $k_{el}(T)$ in CMR manganites. The suppression of k_{el} with increasing doping and its enhancement with higher hybridization or Hund’s coupling emphasize the critical role of electron-lattice and spin-charge interactions in governing heat transport. The theoretical framework captures the essential interplay among these parameters, providing a unified interpretation of thermal transport anomalies in CMR manganites.

4. Conclusion

In this paper, a variational method has been used for the investigation of the electronic thermal conductivity k_{el} at different temperatures for various values of the model parameters like doping x , hybridisation V and J_H parameters. By increasing temperature, we obtain the ferromagnetic transition at $T_c \sim 400$ K in the metallic state. A dip or minimum in thermal conductivity is observed at the ferromagnetic transition temperature ($T_c \sim 400$ K) (Fig. 3). This minimum arises from the complex interplay of lattice dynamics and electron transport during the phase transition. The thermal conductivity k_{el} of colossal magnetoresistance (CMR) manganites shows strong and anomalous temperature dependence with distinct behaviours in the paramagnetic (insulating) and ferromagnetic (metallic) phases. In the low-T metallic phase, it decreases as temperature falls ($dk_{el}/dT < 0$), similar to the typical crystalline behaviour. k_{el} shows an appreciable enhancement as electrons gain mobility and contribute to the thermal transport in the metallic state.

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Submitted 27 January 2026; revised 3 February 2026; accepted 30 May 2026

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Conflict of interest: the authors declare no conflict of interest.