

which is off by an important factor of two from  $S_{\text{Kelvin}}$  (Eq. (11)). The formulations (Mott-Heikes and Kelvin) would be identical if  $\mu \propto T$ , which occurs if the system possesses a ground state degeneracy, and in the classical regime. The high frequency approximation gives a better result than all these and, again in the low temperature limit, to  $\mathcal{O}(T^3)$ ,

$$S^* = T \frac{\pi^2 k_B^2}{3q_e} \frac{d}{d\mu} \ln [\rho_0(\mu) \langle (v_p^x)^2 \rangle_\mu] \big|_{\mu \rightarrow \mu_0}. \quad (13)$$

Other than the neglect of the energy derivative of  $\tau$ , this is the same as the exact result. Hence, ranking the thermopower approximations for non-interacting electrons we have, from worst to best,  $S_{\text{MH}}$ ,  $S_{\text{Kelvin}}$ , and  $S^*$  with the exact result being  $S_{\text{Mott}}$ .

### B. Hubbard model

For intermediate coupling models, the relative rankings of the various approximations can be different. In particular,  $S_{\text{Kelvin}}$  can be superior to  $S^*$ , since the effect of correlations is diluted in the latter by making the assumption of  $\omega \gg U$ , whereas  $S_{\text{Kelvin}}$  retains  $\omega \ll U$ . The sign of the true (i.e. transport) thermopower and the transport Hall constant are expected to flip as we approach half filling in the Hubbard or  $t$ - $J$  models due to the onset of correlations (carriers become holes measured from half filling rather than from a completely filled band). In the case of the  $t$ - $J$  model, the high frequency Hall constant  $R_H^*$  and  $S^*$  do display this behavior<sup>11</sup>. However, for the Hubbard model,  $R_H^*$  and  $S^*$  do not display a sign change<sup>16,17</sup>.  $S_{\text{Kelvin}}$  on the other hand, does appear to show the expected change in sign<sup>16,18</sup>. Further discussion concerning the relative merits of  $S_{\text{Kelvin}}$  and  $S^*$  will be reported later<sup>16</sup>.

### C. NCO and the $t$ - $J$ model

To show the usefulness of  $S_{\text{Kelvin}}$ , we apply it to NCO since (i) we have previously investigated<sup>2</sup> this system while benchmarking  $S^*$ , (ii) the system is intrinsically interesting<sup>1</sup>, and (iii) we can compare different thermopower formulations on equal footing. As discussed<sup>2</sup>, the action in NCO takes place primarily in the cobalt oxide planes where  $d$ -shell spin-1/2 electrons live on a triangular lattice and these strongly interacting 2D electrons can be modeled with the  $t$ - $J$  model. Hence, we exactly diagonalize the  $t$ - $J$  model on a  $L = 12$  site two-dimensional triangular lattice with periodic boundary conditions (cf. Fig. 1e). Note that we only show results for the  $t$ - $J$  model with zero super-exchange interaction ( $J = 0$ ), as the results only weakly depend on  $J$ . To map the  $t$ - $J$  model to NCO we follow Refs. 2 and 4 and give results as a function of electron doping  $x = |1 - n|$  away from half filling ( $n$  is electron number density).

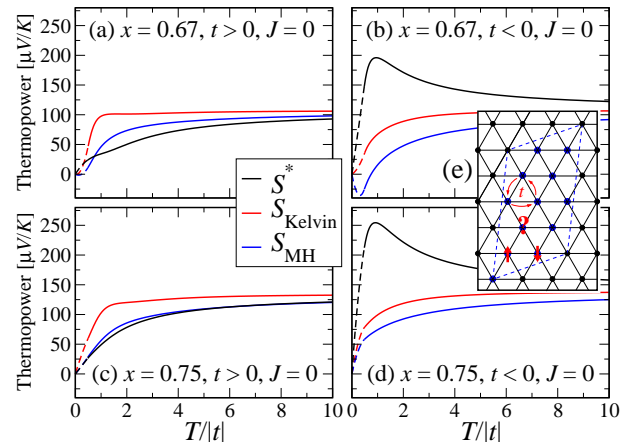


FIG. 1: Thermopower vs.  $T$  for the  $t$ - $J$  model (with  $J = 0$ ) corresponding to NCO in the Curie-Weiss metallic phase near  $x \sim 0.7$ . (a) and (c) correspond to  $x = 0.67$  and  $x = 0.75$  for the NCO system ( $t > 0$ ) while in (b) and (d) the sign of the hopping has been switched to investigate the enhancement expected for frustrated systems. The black, red (light gray), and blue (dark gray) lines are  $S^*$ ,  $S_{\text{Kelvin}}$ , and  $S_{\text{MH}}$ . Finite size effects at low  $T$  are treated in the spirit described previously<sup>2</sup>. At each  $x$ , for  $T$  below an appropriately chosen cutoff temperature  $T_0 = 0.5|t|$ , the thermopower is fit to  $S(T) \rightarrow aT + bT^2$  where  $a$  and  $b$  are obtained from the computed  $S(T_0)$  and  $S'(T_0)$  providing a sensible extrapolation to low  $T$  and plotted as dashed lines. The inset figure (e) depicts the 12-site unit cell.

$S^*$  adequately describes the physics of NCO for  $x > 0.5$  and, in particular the so-called Curie-Weiss metallic phase<sup>2</sup> near  $x \sim 0.7$ . The subject of this work, however, is  $S_{\text{Kelvin}}$ . We see in Figs. 1a and c and 2a, similar to  $S_{\text{MH}}$ ,  $S_{\text{Kelvin}}$  does a good job capturing the physics with minimal computational effort. However,  $S_{\text{Kelvin}}$  does seem to overestimate the thermopower for intermediate temperatures and high dopings as compared to  $S_{\text{MH}}$ . Near  $x \approx 0.7$ ,  $S_{\text{Kelvin}}$  and  $S_{\text{MH}}$  are similar but as  $x$  is decreased the two formulae diverge and for low dopings,  $S_{\text{Kelvin}}$  better captures the physics as it is closer to the more accurate high frequency limit  $S^*$ .

An interesting property of the triangular lattice underlying the physics of NCO is its geometrical frustration<sup>3</sup>, cf. inset Fig. 1e. It was predicted<sup>2,4</sup> that if the sign of the hopping amplitude were flipped to  $t < 0$  the thermopower would be enhanced at low to intermediate  $T$ . We have considered this situation in Figs. 1b and d and 2b. Since the thermopower enhancement for  $t < 0$  compared to  $t > 0$  is largely a consequence of electron-electron interaction it is important to determine whether this effect is captured by  $S_{\text{Kelvin}}$ . We see this enhancement is captured to some extent by  $S_{\text{Kelvin}}$  and  $S_{\text{Kelvin}}$  is better than  $S_{\text{MH}}$  in the large doping region where the enhancement is the greatest, but is missing some of the electron-electron physics at very low  $T$  that is captured by  $S^*$  (as is  $S_{\text{MH}}$ ).