ANALYSIS OF THERMOELECTRIC POWER OF HIGH-T$_C$ SAMPLES USING HUBBARD MODEL

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ABSTRACT

The thermoelectric power (TEP) of Bi$_2$Sr$_2$Ca$_n$Y$_{2-n}$Cu$_2$O$_{8+y}$ (Bi-2212) samples has been extensively studied using Hubbard Model (HM) and Extended Hubbard Model (EHM).

Introduction

Hubbard Model (HM) has been extensively used for the analysis of transport properties of many conducting salts of organic compounds, e.g., N-methylphenazinium-tetra-cyanoquinodimethane (NMP-TCNQ) etc. and high-temperature superconducting (HTC) samples, both of which show M-I transitions [1]. The Hubbard Hamiltonian [1] which has been used in these studies, has the form

$$H = U \sum_i n_{i\uparrow} n_{i\downarrow} - t \sum_{i,\sigma} \left( C_{i,\sigma}^\dagger C_{i+1,\sigma} + H. C. \right),$$

(1)

where

- $U$ is the on-site Coulomb interaction,

- $t$ is the Nearest-neighbour tight-binding transfer integral, $C_{i,\sigma}^\dagger$ ($C_{i,\sigma}$) creates (destroys) an electron of spin $\sigma$ at the $i$-th site and

- $n_{i,\sigma} = C_{i,\sigma}^\dagger C_{i,\sigma}$ is the corresponding number operator with $n_i = n_{i\uparrow} + n_{i\downarrow}$.

The expression for TEP, derived by G. Beni$^1$ and Cooper $et\ al.\ ^2$ using the above Hamiltonian, is given by

$$S_{HM} = \frac{k}{e} \left\{ \ln \left( \frac{1 - p}{2p} \right) - \ln 2 \right\},$$

(2)
In the above expression, $p$ is the hole concentration and $k$ is the Boltzmann Constant. A systematic analysis of the expression (2) leads to the conclusion that for HTS samples Hubbard model has only limited success. One of the shortcomings of this model is the neglect of intermolecular electron repulsion in the Hamiltonian given by equation (1). To take account of the influence of the intermolecular electron repulsion, Kwak et al.\cite{1} have modified the Hamiltonian given by eq. (1) to the form

$$H = U \sum_i n_i \uparrow n_i \downarrow + V \sum_i n_i n_{i+1} - t \sum_{i,\sigma} \left( C_{i,\sigma}^\dagger C_{i+1,\sigma} + H. C. \right),$$

(3)

where $V$ represents the intermolecular electron repulsion. This modified form of the Hamiltonian has been referred to as the Extended Hubbard Model (EHM).

**Results and Discussions**

In some earlier \cite{1} we have reported the details of the derivation of TEP using EHM. The expression for TEP, for HTS samples, has been derived as

$$S_{EHM} = \frac{k}{e} \ln x,$$

(4)

where

$$x = \frac{1 - p}{4pe^{-\beta V}}.$$  

(5)

In the above expression, $\beta = (kT)^{-1}$. In the same paper, the values of $V$ for different insulating samples of Bi-2212 system have also been calculated.

![Fig. 1: TEP vs hole concentration for insulating samples of Bi-2212 system. The dashed and solid curves are the theoretical curves, obtained using eqs. (2) and (4) respectively.](image-url)
Thermo Electric Power of High-TC Samples

Fig. 2: The variation of TEP with p for metallic samples of Bi-2212 system; the dashed and solid curves been been obtained using eqs. (2) and (6) respectively.

In this paper we have analysed the experimental results of TEP of different samples of Bi-2212 system using equation (4). It has been observed that the experimental results of insulating samples of this system can be explained reasonably well using equation (4) [as shown in Fig. 1]. However, the experimental results of the metallic samples can not be explained by this equation.

In order to explain the experimental results of the metallic samples theoretically, we have modified equation (2) phenomenologically. A careful study of equation (2), using best-fit method, shows that the introduction of a linear term in p and a constant to equation (2) can explain the experimental results of metallic samples with good agreement [as shown in Fig. 2]. This modified expression has been found to have the form

\[ S = \frac{k}{c} \left[ \ln \left( \frac{1-p}{2p} \right) - \ln 2 \right] + ap + b, \]  

(6)

where a and b are the fitting parameters which have been identified as

\[ a = \frac{\sqrt{2}}{p_c \ln p_c} \]  

(7a)

and

\[ b = \ln \sqrt{p_c} \]  

(7b)

In equations (7a) and (7b), p_c is an optimal value of p for which T_c is maximum for the corresponding HTS system.
Conclusions

The expression for TEP (eq. 4), derived using EHM, has been found to successfully explain the experimental results of TEP of the insulating samples of different HTS systems.

However, for metallic samples of the same systems TEP has been found to depend on the optimal value of the carrier concentration \( p_c \), which corresponds to the maximum value of \( T_c \) of the system. A theoretical understanding of this study remains to be developed.

REFERENCES