Optimal Spectrum for the Borocarbides
YNi$_2$B$_2$C and LuNi$_2$B$_2$C

S. Manalo$^{1}$ and E. Schachinger$^{2}$

$^{1}$ Institut für Theoretische Physik, J. K. Universität Linz,
Altenbergerstr. 69, A-4040 Linz, Austria

$^{2}$ Institut für Theoretische Physik, Technische Universität Graz,
Petersgasse 16, A-8010 Graz, Austria
E-mail: schachinger@itp.tu-graz.ac.at

(Received November 14, 2000; accepted December 27, 2000)

The concept of an optimal electron–phonon interaction spectral density as an Einstein spectrum which allows to describe all physical properties of a superconductor in an optimal way is developed from Carbotte’s original definition of an optimum spectrum. It is shown, using the borocarbides YNi$_2$B$_2$C and LuNi$_2$B$_2$C as examples, that such a concept is meaningful even for anisotropic systems. An Einstein spectrum is sufficient for clean-limit systems, a 26-peak spectrum is better suited for anisotropic systems with impurities.

1. INTRODUCTION

Conventional superconductors are well described by Eliashberg theory which treats superconductivity as a boson-exchange phenomenon. The dominant feature of this theory is the electron–phonon interaction spectral function $\chi^2F(\omega)$ which can be determined from tunneling experiments or theoretically from band structure calculations. Using such an $\chi^2F(\omega)$ within Eliashberg theory allows to reproduce the superconducting properties of a conventional superconductor within experimental accuracy and this established the phonons as the exchange boson between the two charge carriers building the Cooper pair in conventional superconductors.

Concentrating on isotropic systems Carbotte developed the concept of an optimum spectrum based on earlier work of Leavens and Mitrović and Carbotte. Such a spectrum can be developed from a theorem which states that for a given strength $A = \int_0^\infty d\omega \chi^2 F(\omega)$ of the spectral density
\( x^2 F(\omega) \) the best shape that will maximize the critical temperature \( T_c \) is a delta function spectrum

\[
\Delta^2 F(\omega)_{\text{opt}} = A \delta[\omega - \omega^*(\mu^*)],
\]

with the delta function placed at the frequency \( \omega^*(\mu^*) \) at which the functional derivative \( \delta T_c / \delta \omega^2 F(\omega) \) displays its maximum for a fixed value of the Coulomb pseudopotential \( \mu^* \). Carbotte\(^3\) extended this concept to encompass other physical properties such as \( 2\Delta(0)/k_B T_c \), the zero temperature gap \( \Delta(0) \) to \( T_c \) ratio, and a number of others. This concept establishes that a relation

\[
X = A x(\mu^*)
\]

always exists, where \( X \) stands for \( T_c \), \( 2\Delta(0)/k_B T_c \), etc. and \( x(\mu^*) \) is a universal number determined from Eliashberg theory for each property \( X \) and which varies only slightly with \( \mu^* \).

In essence the optimum spectrum gives information about the phonon frequency important to maximize a certain physical property (such as \( T_c \)) of a conventional superconductor. Such a concept is very appealing and it suggests an expansion to the concept of an optimal spectrum which is again a delta peak spectrum with a delta peak of strength \( A \) at some position \( \omega^*(\mu^*) \) both chosen to reproduce all known properties of a superconductor optimally. Such a spectrum will then provide information on the phonon mode most important for a specific superconductor if an \( x^2 F(\omega) \) cannot be derived from experiment. It can also help to develop an \( x^2 F(\omega) \) in all cases where the phonon density of states \( G(\omega) \) is known.

We would like to put this concept to test using the borocarbides \( \text{LuNi}_2\text{B}_2\text{C} \) and \( \text{YNi}_2\text{B}_2\text{C} \) for which extensive experimental data exist and for which \( G(\omega) \) is known from theoretical work.\(^7, 8\) From experimental data of the upper critical field \( H_{c2} \) which displays a pronounced upward curvature close to \( T_c \) in single crystal\(^7\) and polycrystalline\(^6\) samples we also assume these systems to be anisotropic.\(^10\) Shulga et al.\(^11\) explained this upward curvature of \( H_{c2}(T) \) close to \( T_c \) by considering two bands, one of which being more deeply involved in the transport properties of the compound. The authors utilized an \( s \)-wave electron–phonon Eliashberg formalism and there is growing evidence that the order parameter in \( \text{YNi}_2\text{B}_2\text{C} \) is indeed of \( s \)-wave symmetry.\(^12\) It is interesting to note in passing that concept introduced by Prohammer and Schachinger\(^10\) is effectively a two-band model described by an anisotropic electron–phonon interaction spectral density.\(^13, 14\)

Section 2 of this paper reviews the theoretical background, Sec. 3 discusses the results of our analysis, and, finally, in Sec. 4 our conclusions are drawn.