Angle-Resolved Photoemission Intensity of High Temperature Superconductors Based on the Spin Polaron Formulation

Hannah Rissah E. Forio[1] and Danilo M. Yanga[2]

[1] Physics Division, Institute of Mathematical Sciences and Physics, University of the Philippines- Los Banos,
[2]National Institute of Physics, University of the Philippines- Diliman

Abstract

Spin polaron formulation at finite temperature was used to calculate the angle-resolved photoemission (ARPES) intensity of high-temperature superconductors. In the Matsubara Green's function method, the spin polaron Hamiltonian is the interaction term in S-matrix. In this case, holes are described as spinless fermions (holons) and spins are normal bosons. ARPES intensity calculation considered the imaginary part of the retarded Green's function integrated with a Gaussian instrumental resolution function and with the Fermi-Dirac distribution function.

I. Spin Polaron Formulation

The spin polaron hamiltonian can be expressed as:

$$H_{sp} = \frac{Zt}{\sqrt{N_c}} \sum_{pq} \left[M(\boldsymbol{p}, q) h^+_{\boldsymbol{p}} h_{\boldsymbol{p-q}} z_{\boldsymbol{q}} + h.c. \right]$$

where:
M(**p**,**q**)-the coupling function,

$h^+_p(h_p)$ - holon creation (annihilation) operator,

$z^+_q(z_q)$ -spin wave creation (annihilation) operator

t - transfer integral

Z -coordination number
N_c -normalization factor.

The spin polaron Hamitonian is incorporated into the Matsubara Green's function. The S matrix expansion would yield the finite temperature Green's function containing only the connected, different, Feynman diagrams.

The spin-less hole operator is based on the free Matsubara Green's Function

$$G^0_M(\boldsymbol{p}, ip_n) = [ip_n - \xi_{\boldsymbol{p}}]^{-1}$$

$p_n = (2n+1)\pi/\beta$ -fermion frequencies

$\beta^{-1} = k_B T$

$\xi_p \equiv \Lambda p - \mu$ -single holon energy relative to the Fermi Energy.

Λp -background spin fluctuations energy

μ -chemical potential.

For the free finite temperature spin wave Green's function, the spin wave operator as a linear combination of the Holstein-Primakoff Bosons is defined as: $z_{\boldsymbol{q}} = \lambda_1 a_{\boldsymbol{q}} + \lambda_2 a^+_{-\boldsymbol{q}}$

$$D^0_M(\boldsymbol{q}, i\omega_n) = \lambda_1 \lambda_2 \left[\frac{-2\omega_q}{\omega_n^2 + \omega_q^2} \right]$$

Where:

ω_q is the spin wave energy,

$\omega_n = 2n\pi/\beta$ -Matsubara spin wave frequency

λ_1 and λ_2 are constant coefficients.

II. ARPES Intensity

ARPES measures the imaginary part of the retarded Green's function integrated with a Gaussian instrumental resolution function $F(w, w')$ and with the Fermi-Dirac Distribution function

$$I(\boldsymbol{p}, w) = \frac{n(\varepsilon_p) e^{-\frac{w-\varepsilon_p}{2\gamma^2}}}{\gamma\sqrt{2\pi}} + \int dw' F(w, w') \sum_{\boldsymbol{q}} M^2_{pq} n(w') \left[(N_{\boldsymbol{q}} + n_{\boldsymbol{p-q}})(\delta(w' - \varepsilon_{p-q} + w_q) + (N_{\boldsymbol{q}} - N_{\boldsymbol{p-q}} + 1)(\delta(w' - \varepsilon_{p-q} - w_q) \right]$$

References:

A.S. Alexandrov and N.F. Mott. High Temperature Superconductors and Other Superfluids. Taylor and Francis. UK. 1994.

A.A. Morales, D.M Yanga, Kurihara. Calculation of Entropy and Specific Heat in the Spin Polaron Formulation at Finite Temperature. Journal of Superconductivity: Incorporating Novel Magnetism. Vol. 17. No. 2. Plenum Publishing Corp. pp 283-285. April 2004.

A.A. Morales Jr., DM Yanga, and S. Kurihara. The Hole Spectral Function in the Finite Temperature Green's Function Scheme. Journal of Superconductivity: Incorporating Novel Magnetism, Vol 15, No. 4, pp 277-280. August 2002.

D.M. Yanga and A.A. Morales. A different Theoretical Approach to the Spin Polaron Problem. Plenum Publishing Corporation. pg. 929-931.2000