Contrasting Dynamic Spin Susceptibility Models and their Relation to High Temperature Superconductivity

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Abstract

We compare the normal-state resistivities $\rho$ and the critical temperatures $T_c$ for superconducting $d_{x^2-y^2}$ pairing due to antiferromagnetic (AF) spin fluctuation exchange in the context of the two phenomenological dynamical spin susceptibility models, recently proposed by Millis, Monien, and Pines (MMP) and Monthoux and Pines (MP) and, respectively, by Radtke, Ullah, Levin, and Norman (RULN), for the cuprate high-$T_c$ materials. Assuming comparable electronic bandwidths and resistivities in both models, we show that the RULN model gives a much lower $d$-wave $T_c$ ($\sim 20$K) than the MMP model (with $T_c \sim 100$K). We demonstrate that these profound differences in the $T_c$’s arise from fundamental differences in the spectral weight distributions of the two model susceptibilities and are *not* primarily caused by differences in the calculational techniques employed by MP and RULN. The MMP model, claimed to fit NMR data in YBCO, exhibits substantial amounts of spin fluctuation spectral weight up to an imposed cut-off of 400meV, whereas, in the RULN model, claimed to fit YBCO neutron scattering data, the weight is narrowly peaked and effectively cut-off by 100meV. Further neutron scattering experiments, to explore the spectral weight distribution at all wavevectors over a sufficiently large excitation energy range, will thus be of crucial importance to resolve the question whether AF spin fluctuation exchange provides a viable mechanism to account for high-$T_c$ superconductivity. The large high-frequency boson spectral weight, needed to generate both a high $d$-wave $T_c$ and a low normal-state resistivity, also implies large values, of order unity, for the Migdal smallness parameter, thus casting serious doubt on the validity of the very Migdal approximation on which high-$T_c$ spin fluctuation exchange models are based.

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I. INTRODUCTION

Recently, an increasing, but not uncontroverted amount of experimental data has been shown to be consistent with a $d_{x^2-y^2}$ symmetry of the superconducting order parameter in the cuprate high-$T_c$ superconductors.\(^1\)\(^2\) In early studies of the Hubbard model, Scalapino and co-workers\(^3\) proposed that a pairing state of $d$-wave symmetry can arise due to exchange of antiferromagnetic spin fluctuations.\(^4\) In the model believed to be most relevant to the cuprates, the two-dimensional (2D) Hubbard model, a $d_{x^2-y^2}$ pairing instability was suggested by Bickers et al.\(^5\) and by Moriya et al.\(^6\) Recently, two phenomenological models of the dynamic spin susceptibility $\chi(\mathbf{q}, \omega)$ for the cuprate materials have been developed by fitting an assumed analytical form to experimental data and then using this information to calculate such properties as the resistivity $\rho$ and superconducting transition temperature $T_c$.

The first model, due to Millis, Monien, and Pines, hereafter referred to as MMP, was obtained from fits to nuclear magnetic resonance (NMR) data on $YBa_2Cu_3O_7$ ($YBCO$).\(^7\) This model and modifications thereof were then used to calculate $T_c$ in weak coupling\(^8\) and strong coupling\(^9\)–\(^11\) approaches. Moreover, the resistivity due to spin fluctuation scattering was calculated, both without\(^10\) and with\(^11\) inclusion of leading-order vertex corrections. Also calculated was the suppression of $T_c$ due to non-magnetic impurities.\(^11\) The primary conclusion drawn from the MMP model calculations\(^7\)–\(^11\) was that the NMR data, the temperature-dependent normal-state resistivity, the large superconducting transition temperature $T_c \approx 100K$, and the $T_c$-suppression due to impurities can be consistently accounted for with a single, physically acceptable set of model parameters.

The second model, due to Radtke, Levin, Ullah, and Norman,\(^12\) referred to as RULN hereafter, was obtained from fits to neutron scattering data on $YBCO$.\(^13\) This $\chi(\mathbf{q}, \omega)$ was then used to calculate $T_c$, using a strong coupling approach\(^12\)\(^14\), the resistivity, by variational Boltzmann equation and Fermi-surface-restricted Kubo formalisms\(^12\), and the $T_c$ suppression due to impurities.\(^16\) The primary conclusion drawn from these calculations was that it is essentially impossible to generate a $d$-wave $T_c$ of 90K (or larger) by AF spin fluctuation exchange. In fact, if the effective spin fluctuation coupling constant in the RULN model was adjusted to reproduce the observed magnitude of the normal state resistivity, the resulting $d$-wave $T_c$ was found not to exceed about 10K.

We are thus faced with the obvious controversy that the two different model fits to the dynamic spin susceptibility of $YBCO$ give strikingly different results for the $d$-wave $T_c$ and/or the normal-state transport scattering rates. The MMP model allows to obtain a very high $T_c$, consistent with the cuprates, as well as a rather low resistivity, consistent with recent single crystal data on $YBCO$. The RULN model, on the other hand, gives a much lower upper limit on $T_c$, even for resistivities much larger than the MMP model.

This controversy has led to a number of criticisms on both sides. An early argument\(^10\)\(^12\) concerned the use of different calculational approaches, specifically the use of weak-coupling vs. strong-coupling and approximate semi-analytical Fermi-surface-restricted vs. exact numerical full-zone approaches to calculate $T_c$. However, both groups\(^10\)\(^14\) have now carried
out detailed strong-coupling, full-zone $T_c$ calculations for both models, using fast Fourier transform (FFT) techniques, which allow to include include the full momentum and frequency dependence of the Migdal-Eliashberg equations. In these full-zone results, the order-of-magnitude discrepancy of the $T_c$ values between the two models persists. Clearly, the different magnitudes of $T_c$ are not primarily due to the use of different calculational approaches.

Another objection against the original RULN approach concerned their use of variational Boltzmann or Fermi-surface-restricted Kubo formalisms for calculating the resistivity in the RULN model. These transport formalisms, again, amount essentially to an approximate Fermi-surface-restricted analysis of the relevant full-zone Bethe-Salpeter integral equation. By contrast, in Ref. 11, the resistivity in the MMP model was obtained directly from the numerical full-zone solution of the Bethe-Salpeter equation, without additional approximations. In the present paper, we will show that, again, the discrepancy between the two models is not primarily caused by the use of two different calculational approaches.

What we wish to demonstrate here is that the very different conclusions about attainable $T_c$’s derived from the two models are a direct consequence of the fundamental differences in the assumed dynamic spin susceptibilities $\chi(\vec{q}, \omega)$. We re-emphasize that, even if one uses the same electronic band parameters in both models, the RULN model will still give a substantially lower superconducting $T_c$ than the MMP model. We will show that this difference in $T_c$ arises, ultimately, from the difference in the spectral weight distribution of the two model spin susceptibilities. We therefore conclude that more experimental work is needed, primarily by neutron scattering, to elucidate the frequency dependence of the spin susceptibility $\chi(\vec{q}, \omega)$. Only a complete understanding of the spectral weight distribution, including its full frequency and momentum dependence, will eventually allow us to resolve the issue of whether or not a spin fluctuation pairing mechanism may constitute a viable model of high temperature superconductivity.

On the theoretical side, our analysis of the two different models shows that, in order to produce a large $T_c$ and, at the same time, a sufficiently low normal-state resistivity, the spin fluctuation models, just like any other boson exchange model, must exhibit substantial amounts of spectral weight at a fairly large boson energy scale $\Omega$, as well as a substantial overall Eliashberg coupling parameter $\lambda$, assuming typical bandwidths and Fermi energies $\epsilon_F$ in the cuprates. For such large boson energy scales and coupling strengths, the Migdal smallness parameter $s \equiv \lambda \Omega / \epsilon_F$ is not really small anymore, compared to unity. Thus, Migdal’s “theorem”, the very foundation of current spin fluctuation exchange models, tends to be on rather shaky grounds.

Another important theoretical consequence of having such a large boson energy scale, $\Omega / \epsilon_F \gtrsim 0.1 - 0.2$, is that the conventional mechanism of evading Coulomb interactions by retardation becomes largely inoperative in these types of high-energy boson exchange models. Thus, even though the local, Hubbard-type on-site Coulomb correlations are completely projected away, simply due to the non-s-wave order parameter symmetry, the extended (e.g. nearest neighbor) part of the Coulomb interaction potential can be quite effective in suppressing the spin-fluctuation-mediated $d$-wave $T_c$. Current spin fluctuation models, including the MMP model, have so far entirely ignored the extended part of the Coulomb interaction potential and may thus be severely overestimating the actual $d$-wave $T_c$ values which can be ultimately achieved via a spin fluctuation exchange mechanism.
In passing, we should also comment briefly on the on-going controversy concerning impurity effects. Monthoux and Pines\textsuperscript{11} claimed that the suppression of $T_c$ due to pairbreaking by non-magnetic impurities is much weaker than would be indicated by Abrikosov-Gor’kov\textsuperscript{15} (AG) theory. Radtke \textit{et al.}\textsuperscript{16} on the other hand claimed that the suppression of $T_c$ due to non-magnetic impurities in both models is roughly in agreement with a strong-coupling version of AG theory proposed by Millis \textit{et al.}\textsuperscript{19} At this point, we can only emphasize, again,\textsuperscript{16} that the two models are indeed quite consistent in that aspect. The differences claimed to exist by Monthoux and Pines\textsuperscript{11} are entirely a matter of different calculational approaches for evaluating the impurity scattering rate from the input impurity potential strength, using either the $t$-matrix\textsuperscript{11} or leading-order Born\textsuperscript{16},\textsuperscript{11} approximation. If the calculated impurity-induced $T_c$-suppression is plotted as a function of the calculated impurity scattering rate (rather than as a function of the input impurity potential strength), then both approaches, Born and $t$-matrix, give quite similar results. That is, for a given magnitude of impurity scattering rate, one obtains essentially the same $T_c$-suppression, regardless of how that scattering rate was calculated from the input impurity potential. The important point to remember here is that it is the impurity scattering rate, not the input potential strength, which is measured experimentally via the impurity-induced ”residual” resistivity.

The remainder of the paper is organized as follows:

In Section II, we introduce the two AF susceptibility models, proposed by MMP\textsuperscript{7} and RULN\textsuperscript{12}, and summarize the different approaches used by Monthoux and Pines\textsuperscript{9–11} (referred to as MP, hereafter) and by RULN\textsuperscript{12} in determining the electronic band parameters and in calculating transport properties, for their respective models.

In Section III, we discuss in some detail the underlying physical assumptions on which, implicitly, the different approaches for estimating the band parameters and for calculating transport properties are based. We then give a direct comparison of the different transport formalisms, for the case of the MMP model, and discuss the limits of applicability of both the Fermi-surface-restricted Boltzmann and the full-zone Bethe-Salpeter formalisms, and of the underlying Migdal approximation.

In Section IV, we discuss the origin of the differences in the $d$-wave pairing $T_c$’s extracted from the two models. We show that the substantial differences in the $T_c$’s of the two models are, ultimately, not due to the differences in the assumed bandwidth parameters or in the transport formalism used to estimate the coupling parameter. By means of a McMillan-Allen-Dynes analysis\textsuperscript{20,21} we demonstrate that the primary cause for the differences in $T_c$ lies in the different spectral weight distributions of the two model spin susceptibilities.

Concluding remarks are presented in Section V.

\textbf{II. MODEL SUSCEPTIBILITIES, BAND AND COUPLING PARAMETERS}

We start by describing the two models. The MMP model is a fit designed to describe NMR data in $YBCO$, based on a susceptibility spectral function of the analytical form
\[
\text{Im}\chi_{\text{MMP}}(\vec{q}, \omega + i0^+) = \frac{\chi_0\omega/\omega_{sf}}{(1 + \xi^2|\vec{q} - \vec{Q}|^2 + (\omega/\omega_{sf})^2)} \Theta(\Omega_c - |\omega|) \tag{1}
\]

where \(\vec{Q} = (\pi/a, \pi/a)\) and \(\vec{q} \equiv (q_x, q_y)\) is in the 1st quadrant of the two-dimensional (2D) square lattice Brillouin zone and a frequency cut-off taken as \(\Omega_c = 400\text{meV}\). In the most recent version of the model, proposed by Monthoux and Pines\textsuperscript{11}, hereafter referred to as MP-II, the other parameter values are, as given in Table II of that paper\textsuperscript{11} for a 25% hole doping concentration,

\[
\omega_{sf} = 14\text{meV}, \quad \xi/a = 2.3, \quad \chi_Q = 75\text{eV}^{-1}. \tag{2}
\]

where \(a \approx 3.8\text{Å}\) denotes the 2D \(\text{CuO}_2\) square lattice constant. Note, that in MP-II\textsuperscript{11}, the resistivity as a function of temperature \(T\) was actually calculated by using a \(T\)-dependent \(\omega_{sf}, \chi_Q, \xi\) as defined in Eqs. (37), (27) and (5b) of that paper\textsuperscript{22} respectively, that is, in the notation of MP-II\textsuperscript{11}

\[
\omega_{sf}(T) = 9.5\text{meV} + 4.75 \times 10^{-2}(\text{meV/K}) \times T
\]

\[
\chi_Q(T) = \frac{\chi_0 \Gamma_{sf}}{\pi\omega_{sf}(T)}
\]

\[
\xi(T)/a = \left[\Gamma_{sf}/\pi \beta^{1/2} \omega_{sf}(T)\right]^{1/2} \tag{3}
\]

with \(\Gamma_{sf} = 1.3\text{eV}, \chi_0 = 2.6\text{eV}^{-1}\) and \(\beta = 32\). At \(T \approx 100K\), these \(T\)-dependent values Eq.(3) agree to within a few percent with those of Eq.(2), taken from MP-II’s Table II. In the following we will use exclusively the \(T\)-dependent values of \(\omega_{sf}, \xi/a, \) and \(\chi_Q\) from Eq.(3).

The RULN model susceptibility, designed to fit neutron scattering data in \(\text{YBa}_2\text{Cu}_3\text{O}_7\), is given by\textsuperscript{12}

\[
\text{Im}\chi_{\text{RULN}}(\vec{q}, \omega + i0^+) = C\left[\frac{1}{1 + J_0(\cos(q_xa) + \cos(q_ya))}\right]^2
\]

\[
\times \frac{3(T + 5)\omega}{1.05\omega^2 - 60|\omega| + 900 + 3(T + 5)^2} \Theta(\Omega_c - |\omega|) \tag{4}
\]

with the temperature \(T\) and excitation energy \(\omega\) measured in meV, a cut-off \(\Omega_c = 100\text{meV}\), a constant \(J_0 = 0.3\) and a prefactor \(C = 0.19\text{eV}^{-1}\).

In either model, the spin-fluctuation-mediated electron-electron interaction potential \(V(\vec{q}, \omega)\) is then obtained by multiplying \(\chi(\vec{q}, \omega)\) by a coupling constant \(g^2\), that is

\[
V(\vec{q}, \omega) = g^2\chi(\vec{q}, \omega) = g^2 \int_{-\infty}^{+\infty} \frac{d\omega'}{\pi} \text{Im}\chi(\vec{q}, \omega' + i0^+) \frac{1}{\omega' - \omega} \tag{5}
\]

for transfer of momentum \(\vec{q}\) and complex frequency \(\omega\). To calculate superconducting \(T_c\)’s and normal state conductivities, using standard diagrammatic and/or transport theory approaches, this interaction potential is combined with a 2D tight-binding electron bandstructure

\[
\epsilon_k = -2t_1[\cos(ak_x) + \cos(ak_y) - 2t \cos(ak_x) \cos(ak_y) - \epsilon] \tag{6}
\]
with a chemical potential $\mu \equiv 2e \times t_1$ and 1st and 2nd neighbor hopping matrix elements $t_1$ and $t_2 \equiv t \times t_1$, respectively. To fix the ratios $t \equiv t_2/t_1$ and $e \equiv \mu/2t_1$, both RULN and, subsequently, MP-II used the Fermi surface shapes and Fermi surface volumes found in LDA bandstructure calculations, which are consistent with angle-resolved photoemission experiments. In the case of $YBa_2Cu_3O_{6.75}$, considered by RULN, this gave $t \approx +0.45$, working in the hole picture, and a $\mu$ value which corresponds to a hole doping concentration, measured from half-filling, of $x = 0.18$ holes per $Cu$-site, that is, a total hole concentration of $n_h \equiv 1 + x = 1.18$ holes per $Cu$-site. MP-II adopted the same value for $t$, but assumed a somewhat larger hole doping concentration of $x = 0.25$ holes per $Cu$-site, to correspond to the case of $YBa_2Cu_3O_{6.9}$. However, MP-II and RULN then employed two very different approaches to determine the bandwidth $8t_1$ and the spin fluctuation coupling constant $g^2$.

MP-II adjusted $t_1$ to match roughly the calculated LDA bandstructure $\epsilon^*_{\vec{k}}$ near the Fermi surface, giving a $t_1 \approx 250$meV for $YBCO$. They then adjusted their $g^2$ to give a superconducting $d$-wave $T_c$ of about 100K, as obtained from solutions of the full-zone $\vec{k}$- and $\omega$-dependent linearized Eliashberg equations with the spin-fluctuation-mediated interaction potential $V(\vec{q}, \omega)$ from Eqs.(1), (3) and (5). This gave a value of $g = 0.64$eV. Using the same interaction potential, with the same $g^2$ and $t_1$, they then solved the full-zone $\vec{k}$- and $\omega$-dependent Bethe-Salpeter equation in the normal-conducting state to calculate the $T$-dependent resistivity due to spin fluctuation scattering. This calculated model resistivity was shown to be in reasonable agreement with the experimental data on $YBa_2Cu_3O_{6.9}$.

Assumed input values and calculated results for the MP-II model parameters are summarized in the last column of our Table I.

RULN, on the other hand, tried to base their parameter values $t_1$ and $g^2$ entirely on experimental DC and optical conductivity data, rather than $T_c$ and LDA bandstructure results. Their starting point are Drude model fits to the measured low-frequency optical conductivity of $YBa_2Cu_3O_{6.75}$, of the form

$$\text{Re} \sigma(\omega) = \frac{\omega_{p,D}^2}{4\pi} \frac{\tau_D}{1 + \tau_D^2 \omega^2}$$

(7)

parametrized by a Drude plasma frequency $\omega_{p,D}$ and a Drude relaxation time $\tau_D$. Having fixed $t \equiv t_2/t_1$ and the band-filling, RULN determined their $t_1$ by equating the experimental Drude plasma frequency $\omega_{p,D}$, with the "bare" (non-interacting band) plasma frequency

$$\omega_{p,0}^2 = 2N_L \frac{4\pi e^2}{a_\perp} \int \frac{d^2k}{(2\pi)^2} \delta(\epsilon_{\vec{k}}) v_x^2(\vec{k})$$

(8)

where

$$v_x(\vec{k}) \equiv \frac{\partial}{\partial k_x} \epsilon_{\vec{k}},$$

(9)

$a_\perp$ is the $c$-axis lattice spacing (perpendicular to the $CuO_2$ layers), $N_L$ is the number of $CuO_2$ layers per 3D unit cell, and the prefactor 2 arises from the electron spin degeneracy. Note here that, for fixed $t$, $a$, $a_\perp$ and band-filling, $\omega_{p,0}^2$ is proportional to $N_L \times t_1$. Setting $\omega_{p,0}$ equal to the experimental $\omega_{p,D} = 0.97(\pm 0.05)$eV for $YBCO$, RULN thus obtained $t_1 = 80(\pm 10)$meV, as listed in the column 1 of our Table I. However, in this original estimate, RULN had
assumed an incorrect value of $N_L = 1$, corresponding to only one CuO$_2$ layer per unit cell. With the correct number of $N_L = 2$ CuO$_2$ layers per unit cell in YBCO, one obtains a revised estimate for $t_1$ which is reduced from the original value by a factor of 2, i.e. $t_1 = 40$meV, since $\omega_{p,0}^2 \propto N_L \times t_1$. Our following discussion will be based on these corrected values for $N_L$ and $t_1$, shown in column 2 of Table I.

Having thus fixed $t_1$, RULN then determined their spin fluctuation coupling constant $g^2$ by equating the experimentally determined $T$-dependent Drude relaxation rate $1/\tau_D$, from Eq.(7), with the calculated ”bare” relaxation rate $1/\tau_0$, given by

$$1/\tau_0 \equiv 2\pi T \times \lambda_{tr,0} = 2\pi T \times 2 \int_0^{\infty} \frac{d\omega}{\omega} \alpha_{tr}^2 F(\omega) \phi(\omega/T)$$

where $\phi(x) = [(x/2)/\sinh(x/2)]^2$ in the variational Boltzmann and $\phi(x) = x/\sinh(x)$ in the Fermi-surface-restricted Kubo formalism for $x \equiv \omega/T$. The transport spectral function $\alpha_{tr}^2 F(\omega)$, as given by Allen and Glazman, is

$$\alpha_{tr}^2 F(\omega) = \frac{a^2 \int \frac{d\epsilon_{\vec{k}}}{(2\pi)^3} \int \frac{d\epsilon_{\vec{k}'}}{(2\pi)^3} \delta(\epsilon_{\vec{k}})\delta(\epsilon_{\vec{k}'}) (v_x(\vec{k}) - v_x(\vec{k}'))^2 \Im V(\vec{k} - \vec{k}', \omega + i0^+) \pi \int \frac{d\epsilon_{\vec{k}}}{(2\pi)^3} \delta(\epsilon_{\vec{k}})}{2\nu_x^2(\vec{k})}$$

From $\tau_0$ and $\omega_{p,0}$, the DC resistivity in this formalism is calculated as

$$\rho = \frac{4\pi}{\omega_{p,0}^2 \tau_0} = \frac{8\pi^2 T \lambda_{tr,0}}{\omega_{p,0}^2}$$

Notice for the following that, as calculated from Eqs. (8-12), for fixed $T$, $t$, $a$ and band-filling, $1/\tau_0$ and $\lambda_{tr,0}$ scale proportional to $g^2/t_1$, whereas $\rho$ scales proportional to $g^2/t_1^2$.

By matching $1/\tau_0$, calculated from Eqs. (8-11), in the Fermi-surface-restricted Kubo formalism, to a conservative upper limit on the then available experimental $1/\tau_D$ data in the cuprates, taken between about 120K and 350K, RULN thus inferred an upper limit for the coupling constant, $g^2 = 0.533$eV$^2$, based on their incorrect value of $t_1$ estimate of 80meV, as shown in the column 1 of Table I. Using the corrected value of $t_1 = 40$meV, this $g^2$ value also has to be corrected downward, by a factor of 2, to $g^2 = 0.267$eV$^2$, as shown in column 2 of Table I, in order to maintain the same values of $1/\tau_0$ and $\rho$ as in the original RULN paper. Note that, given the band parameters, the foregoing procedure of determining $g^2$ is essentially equivalent to adjusting $g^2$ so as to roughly fit the calculated resistivity from Eq.(12) to the (upper limit) experimental resistivity

$$\rho \equiv 1/\text{Re}\sigma(0) = \frac{4\pi}{\omega_{p,D}^2 \tau_D}$$

From standard transport theory, it is well-known that neither $\omega_{p,0}$ nor $\omega_{p,D}$ nor $\tau_0$ and $\tau_D$ are necessarily the same. RULN’s basic approach of simply equating first $\omega_{p,0} = \omega_{p,D}$, and then $\tau_0 = \tau_D$, to extract the bandwidth 8$t_1$, and, respectively, $g^2$ from the optical conductivity data, is thus based on several simplifying assumptions. This will be discussed in more detail in Section III of this paper.

By solving the full-zone $k$- and $\omega$-dependent linearized Eliashberg equations for the RULN model, with $g^2$ and $t_1$ values extracted from the optical data, one then obtains an upper-limit
$d$-wave $T_c$, from Fig. 1, of about 11K, as shown in columns 1 and 2 of Table I. An important point to notice here is that RULN based their parameter estimates on the then available transport data on early YBCO samples which had much larger in-plane resistivities than the more recently reported samples. Consequently, RULN’s model parameters give a resistivity for their model which is significantly larger than MP-II’s $\rho$ values for the MMP model or the recent experimental $\rho$ data on YBa$_2$Cu$_3$O$_{6.9}$, used by MP-II for comparison to their MMP model results.

Specifically, using RULN’s $\omega_{p,0} = 0.97$ eV and their upper limit for $\lambda_{tr,0} \equiv 1/(2\pi T \tau_0) \sim 0.52$ (approximately constant for $T > 120$K) RULN have a relaxation rate $1/\tau_0 = 2\pi \lambda_{tr,0} T \sim 56$ meV and a resistivity of about $450 \mu\Omega \text{cm}$ at $T = 200$K, as shown in columns 1 and 2 of Table I for the Fermi-surface-restricted Kubo formalism. By contrast, MP-II obtained about 64 $\mu\Omega$ cm at 200K, from their solution of the full Bethe-Salpeter transport equation, consistent with the in-plane-averaged resistivity of YBa$_2$Cu$_3$O$_{6.9}$. From the width (HWHM) of MP-II’s Re$\sigma(\omega)$-results at 200K, shown in Fig. 13 of MP-II, we can also infer a rough estimate for the calculated Drude relaxation rate $1/\tau_D$ and Drude plasma frequency $\omega_{p,D}$ in the MMP model, namely $1/\tau_D \sim 12$ meV and, from Eq. (13), $\omega_{p,D} = (4\pi/\rho \tau_D)^{1/2} \sim 1.2$ eV, as shown in the last column of Table I.

Thus, for the respective model parameters used, MP-II and RULN obtain or, respectively, assume comparable values for the Drude plasma frequency, $\omega_{p,D} \sim 1$ eV, consistent with the experimental data. However, the Drude relaxation rate and the resistivity of MP-II are smaller than those of RULN by factors of about 5-7. And yet, the $d$-wave $T_c$ of MP-II, is larger than that of RULN by a factor of about 9. We are thus called upon to explain why $T_c$ in the RULN model comes out so much smaller than in the MMP model, even for parameter values giving the RULN model a substantially larger resistivity than the MMP model.

III. MASS RENORMALIZATION, TRANSPORT FORMALISMS, AND MIGDAL PARAMETERS

In the present section, we will discuss in some detail the major calculational differences, between RULN and MP-II, in their determination of the bandwidth and in their formalism for obtaining the resistivity. We will elucidate the underlying assumptions upon which the different approaches are based and point out some of the potential short-comings of either approach.

First of all, regarding the bandwidth determination, recall that the RULN estimate for the bandwidth $8t_1 \equiv 0.32$ eV, corresponds to a non-interacting plasma frequency $\omega_{p,0}$ which equals the observed Drude value for YBCO, $\omega_{p,D} \equiv 0.97$ eV (see columns 1 and 2, Table I). This bandwidth is a factor of 6.25 smaller than the LDA-based $8t_1 = 2.0$ eV of MP-II. The latter corresponds, by Eq. (8), to a non-interacting plasma frequency $\omega_{p,0}^{(LDA)} \approx 2.42$ eV, at the RULN’s assumed band-filling $n_h = 1.18$ (see column 3, Table I). It is presently not known whether the observed optical mass enhancement
\[ Z_D \equiv \left( \frac{\omega_{p,0}^{(LDA)}}{\omega_{p,D}} \right)^2 \sim 6.25 \quad (14) \]

is caused primarily by spin fluctuations or by non-spin-fluctuation effects. It seems likely that both contributions are present and non-negligible in the cuprates, that is

\[ Z_D = Z_{nsf} \times Z_{sf} \quad (15) \]

with \( Z_{sf} \) denoting a spin fluctuation and \( Z_{nsf} \) a non-spin-fluctuation contribution, respectively. In equating the observed Drude plasma frequency \( \omega_{p,D} \) with their "bare" model plasma frequency \( \omega_{p,0} \), RULN thus implicitly made the following simplifying assumptions:

Firstly, they assumed that all the non-spin-fluctuation-induced mass enhancement effects can be essentially accounted for by using, as input into the spin fluctuation calculation, an effective bandwidth \( 8t_1 \) and an effective spin fluctuation coupling constant \( g^2 \) into which all non-spin-fluctuation renormalization effects have been absorbed. Thus

\[
Z_{nsf} = \left( \frac{\omega_{p,0}^{(LDA)}}{\omega_{p,0}} \right)^2 \\
Z_{sf} = \left( \frac{\omega_{p,0}}{\omega_{p,D}} \right)^2.
\]

where \( \omega_{p,0} \) is the effective "bare" plasma frequency, corresponding to RULN’s effective \( t_1 \) via Eq.(8).

Secondly, RULN assumed that the observed \( Z_D \) is dominated by non-spin-fluctuation effects, i.e. arises from local Coulomb (and possibly other, such as electron-phonon) interactions excluding the effect of spin fluctuations, whereas the spin fluctuation contribution is negligible, that is

\[
Z_D \cong Z_{nsf} \\
|Z_{sf} - 1| \ll 1
\]  

(17)

Given these two assumptions, the effective bandwidth and effective coupling constant can be inferred directly from the experimental data for \( \omega_{p,D} \) and \( 1/\tau_D \), as was done by RULN. Note however, that the term "bare," in the context of the RULN approach, should then be understood to mean only "bare of renormalizations due to spin fluctuations", and not "bare of all residual interactions beyond LDA”.

Recall here that, in conventional Fermi-surface-restricted transport theory, the width (HWHM) of the Drude peak, \( 1/\tau_D \), and its integrated spectral weight, \( \omega_{p,D}^2 \), are related to \( \tau_0 \) and \( \omega_{p,0} \) as follows:

\[
\omega_{p,D}^2 \cong \frac{\omega_{p,0}^2}{Z_{sf}} \\
\tau_D \cong \tau_0 \times Z_{sf}.
\]

(18)

Thus, \( 1/\tau_D \) and \( \omega_{p,D}^2 \) are both renormalized by \( Z_{sf} \) in such a way that \( Z_{sf} \) cancels out in the DC resistivity

\[
\frac{4\pi}{\omega_{p,D}^2 \tau_D} = \rho = \frac{4\pi}{\omega_{p,0}^2 \tau_0}.
\]

(19)
as already implied by Eqs.(12) and (13). One can therefore indeed calculate the DC resistivity \( \rho \equiv 1/\sigma(0) \) directly from \( \omega_{p,0}^2 \) and \( 1/\tau_0 \), as assumed by RULN in Eq.(12). However, one may not equate \( \omega_{p,0} \) with the observed \( \omega_{p,D} \), nor \( \tau_0 \) with \( \tau_D \), unless the conditions of Eq.(17), i.e. \( |Z_{sf} - 1| \ll 1 \) are met, a point on which we elaborate further below.

As far as spin- and non-spin-fluctuation mass enhancements are concerned, MP take the extreme opposite point of view: They implicitly assume that essentially all of the observed Drude mass enhancement \( Z_D \) is generated by the spin fluctuations and that all non-spin-fluctuation effects are negligible, that is, in Eq.(15),

\[
Z_D \equiv Z_{sf} \\
|Z_{nsf} - 1| \ll 1
\]  

Given that assumption, one should compare the experimental data only to the calculated model Drude relaxation rate \( 1/\tau_D \) and calculated Drude plasma frequency \( \omega_{p,D} \), which fully include all spin-fluctuation-induced mass renormalization effects. To estimate the values of \( 1/\tau_D \) and \( \omega_{p,D} \) given in Table I for the MMP model, we have thus extracted \( 1/\tau_D \) directly from the Drude peak width (HWHM) of the Bethe-Salpeter solution for the optical conductivity \( \sigma(\omega) \), shown in Fig. 13 of MP-II. Using the \( \rho \) value (at \( T = 200K \)) from Fig. 12 of MP-II, we have then obtained \( \omega_{p,D} \) from Eq.(13), i.e. by \( \omega_{p,D} = (4\pi/\rho_0 \tau_D)^{1/2} \). The resulting MMP model value for \( \omega_{p,D} \), as discussed above, is in rough agreement with the experimental data on YBCO.

Physically, both the RULN and the MP treatment of the quasi-particle mass enhancement raises some concerns. As far as the RULN approach is concerned, their model assumption of simply absorbing all non-spin-fluctuation effects into an effective \( t_1 \) and an effective \( g^2 \) clearly needs to be re-examined and justified within the framework of a microscopic theory. Also, for the \( t_1 \) and \( g^2 \) estimates given in column 2 of Table I, the spin fluctuation contribution \( Z_{sf} \) to the overall mass enhancement \( Z_D \) may not really be negligible. Namely, given the spin-fluctuation-mediated interaction potential, Eq.(5), one can get a rough estimate of \( Z_{sf} \) from the self-consistently calculated single-particle self-energy \( \Sigma(k, \omega + i0^+) \) due the spin fluctuations as follows:

\[
Z_{sf} \sim 1 - \left\langle \frac{\partial}{\partial \omega} \text{Re} \Sigma(k, \omega + i0^+)|_{\omega=0} \right\rangle_{FS} \sim 1 + \lambda_Z > 1,
\]  

where \( \langle \ldots \rangle_{FS} \) denotes a suitable Fermi surface average and \( \lambda_Z \) is the dimensionless Eliashberg coupling parameter

\[
\lambda_Z = 2 \int_0^\infty \frac{d\omega}{\omega} \alpha_Z^2 F(\omega),
\]  

obtained from the Eliashberg spectral function of the spin-fluctuation-mediated interaction potential

\[
\alpha_Z^2 F(\omega) = \frac{a^2 \int d^2k \int d^2k' \delta(\epsilon_k) \delta(\epsilon_{k'}) \text{Im}V(\mathbf{k} - \mathbf{k}', \omega + i0^+)}{\pi \int \frac{d^2k}{(2\pi)^2} \delta(\epsilon_k)}
\]  

(23)
In the RULN model with the parameter values of columns 1 or 2, Table I, and temperatures \( T \gtrsim 200K \) one finds \( \lambda Z \sim 0.8 - 1.1 \) and thus \( Z_{sf} \sim 1.8 - 2.1 \) which is not a negligible factor, contrary to Eq.(17).

To infer both \( t_1 \) and \( g^2 \) from the transport and optical data, one should therefore really carry out a calculation for the full dynamical conductivity \( \sigma(\omega) \) in the RULN model, including all spin-fluctuation-induced mass-renormalization effects, and adjust both \( t_1 \) and \( g^2 \), simultaneously, such that the calculated \( 1/\tau_D \), from the Drude peak width, and the calculated \( \omega_{p,D} \), from \( \omega_{p,D} = (4\pi/\rho\tau_D)^{1/2} \), Eq.(13), both match the experimental values. Such an approach would likely give substantially larger estimates for both \( t_1 \) and \( g^2 \) if one assumes as input RULN’s original experimental \( \omega_{p,D} \) and (upper-limit) \( \rho \) values, as given in columns 1 and 2 of our Table I.

However, if one uses the more recent, much lower \( \rho \) data for \( YBCO \), the original RULN procedure would give a much smaller \( g^2 \) and \( \lambda Z \) estimate, with about the same \( t_1 \), as in column 2 of Table I. The resulting \( Z_{sf} \) would then indeed be close to unity, i.e. the conditions of Eq.(17) would be satisfied. So, based on the more recent, lower \( \rho \) data, the original RULN approach could actually be justified, at least as far as consistency with the underlying assumptions about \( Z_{sf} \) is concerned. It is obvious from Fig.1, that the resulting \( T_c \), based on these lower \( \rho \) values, would be substantially below 11K, due to the smaller \( g^2 \) value. So, if one were to use the RULN model susceptibility together with the most recent transport data for \( YBCO \) as input into the a fully self-consistent calculation of \( \sigma(\omega) \), including all spin-fluctuation-induced mass-renormalization effects, one would ultimately find about the same \( t_1 \), but a substantially smaller value for \( g^2 \) and \( T_c \) than the original RULN estimates stated in columns 1 and 2 of our Table I.

As far as the MP approach is concerned, there is no good justification for assuming that non-spin-fluctuation contributions to the mass enhancement are negligible. As recently demonstrated explicitly for the case of electron-phonon coupling, non-spin-fluctuation contributions can significantly suppress the \( d \)-wave \( T_c \), if \( |Z_{nsf} - 1| \sim \mathcal{O}(1) \). In the MMP model, one is then forced to assume a substantially larger spin fluctuation coupling \( g^2 \) than was used in MP-II, in order to maintain a \( T_c \sim 100K \). This, in turn, will cause a larger model resistivity in the normal state, above \( T_c \). Thus, if substantial non-spin-fluctuation contributions to the the mass enhancement are present, the agreement between the MMP model results and the experimental transport data becomes somewhat questionable.

A second major difference between MP and RULN lies in their calculational approaches for obtaining the resistivity. Originally, MP had calculated the optical conductivity \( \sigma(\omega) \) diagrammatically from the self-consistent single-particle Greens function, in the simplest single-loop approximation, without vertex corrections. Subsequently, in MP-II they tried to improve upon that approach by including vertex corrections to the current correlation function, at the level of a Bethe-Salpeter ladder approximation. Their solution of this "full-zone" Bethe-Salpeter equation was done numerically, without further approximations, including the full \( k \)- and \( \omega \)-dependence of the current vertex function.

RULN, on the other hand, relied on the variational Boltzmann and Fermi-surface-restricted Kubo formalisms outlined above. It is well-known that the semi-classical Boltzmann equation can be derived, under certain simplifying conditions, by an approximate Fermi-surface-restricted analysis of the full-zone Bethe-Salpeter equations. These simplifying conditions are indeed well obeyed by conventional wide-band electron-phonon
However, as discussed further below, it is not clear whether these simplifying
conditions are also satisfied for the spin fluctuation models under consideration here.

To test the various transport formalisms, we have calculated the resistivity for the case of
the MMP model, using both of the Fermi-surface-restricted approaches, and compared
to the results obtained by MP-II from numerical solutions of the full-zone Bethe-Salpeter
equation, as shown in their Fig.12, with the $T$-dependent spin fluctuation parameters
given by Eq.(3). The results of this comparison are shown in our Fig. 2. As suggested in
MP-II, we find that both the variational Boltzmann and the Fermi-surface-restricted Kubo
formalism, as used by RULN, do indeed overestimate the resistivity, compared to the Bethe-
Salpeter results. On the other hand, the overestimate, being about a factor of 1.7 for the
Fermi-surface-restricted Kubo formalism at 200 K, is by no means as large as was implied
in MP-II. For the variational Boltzmann formalism, the overestimate is somewhat larger,
about a factor of 2.1 relative to the Bethe-Salpeter results at $T=200$K. Note here, that the
g$^2$ estimate obtained by RULN for their model was based on resistivity calculations in the
Fermi-surface-restricted Kubo formalism.

Several causes could, potentially, contribute to the differences between the full-zone
Bethe-Salpeter and the Fermi-surface-restricted variational Boltzmann results shown in Fig.
2. First of all, there is a numerical issue, having to do with the method used in MP-II
to calculate the optical conductivity $\sigma(\omega)$ in the real-frequency domain. In MP-II, the
numerical solution of the Bethe-Salpeter equation and the subsequent calculation of the
current-current correlation function $C(\omega) \equiv i\omega \sigma(\omega)$ were actually carried out in the Matsubara
imaginary-frequency domain. The Vidberg-Serene Padé-approximant technique was then used to analytically continue the imaginary-frequency data $C(i\omega_m)$, from imaginary frequencies $i\omega_m \equiv 2\pi miT$ into the real-frequency correlation function $C(\omega + i0^+)$, defined on the real-$\omega$ axis. This analytical continuation procedure is mathematically equivalent to an inverse Laplace transform and well-known to be numerically highly unstable. That is, even very small numerical errors in the imaginary-frequency input data $C(i\omega_m)$, for example due to finite cut-offs in the Matsubara frequency summations, can produce large errors in the real-frequency output data $C(\omega + i0^+)$. This problem tends to become particularly severe at higher temperatures when the smallest non-zero Matsubara frequency off the real axis, $i\omega_1$, becomes comparable or larger in magnitude than the characteristic frequency scale one is trying to resolve on the real-$\omega$ axis. For example, in the MP-II calculation at $T=200$K, $\omega_1 = 2\pi T = 108$meV which is more than 4 times larger than the width of the real-frequency spectral feature, the Drude peak width $2/\tau_D \approx 24$meV, to be resolved. It is not clear what level of numerical accuracy was actually achieved in the analytical continuation of MP-II.

Another potential source for discrepancies between variational Boltzmann and full-zone
Bethe-Salpeter approach lies in the two-step approximation which is being used to derive the
former from the latter. The first approximation step consists of restricting the analysis
of the full Bethe-Salpeter ladder equation to the Fermi surface. This step reduces the
Bethe-Salpeter equation to the linearized semi-classical Boltzmann transport equation. The
second step is then to employ a simple variational ansatz to obtain an approximate analytical
solution to the Boltzmann equation, which leads to our Eqs. (8-12).

The error from the second approximation step, the variational ansatz, may become appreciable when the temperature falls below the characteristic boson energy scale $\Omega$. For example, in the case of acoustic phonon exchange, the error is found to cause overestimates
in $\rho$ as large as 30% at temperatures of about $\frac{1}{2}$ of the Debye phonon energy. In the case of the MMP model, the relevant boson energy scale $\Omega$ is of the order of $100 - 150$ meV, as estimated e.g. by the spin fluctuation spectral moments $\langle \omega^p \rangle^{1/p}_Z$ listed in the last column of Table I and defined below. This is about a factor of $6 - 9$ larger than $T$ at $T = 200$ K and could therefore cause errors due the variational ansatz to be of similar ($\sim 30\%$) magnitude. However, in the case of the RULN model, the respective frequency moments (see Table I columns 1-4) are about $2.5 - 3$ times smaller, thus substantially reducing the error due to the variational ansatz for that model.

The first approximation step, reducing the Bethe-Salpeter to the linearized semi-classical Boltzmann equation, requires that the dimensionless Migdal parameter

$$s \equiv \frac{\lambda Z}{\epsilon_F}$$

be small compared to unity. Here, $\lambda Z$ is the Eliashberg parameter, from Eq.(22), $\epsilon_F$ is the Fermi energy, measured from the nearest band edge, and $\Omega$ is again the characteristic boson energy scale. A reasonable order of magnitude for $\Omega$ can be estimated e.g. by taking a low-order frequency moment of the Eliashberg spectral function $\alpha^2 Z F(\omega)$, Eq.(23), or of the transport spectral function $\alpha^2_{tr} F(\omega)$, Eq.(11), that is, e.g.

$$\Omega \sim \langle \omega^p \rangle^{1/p}_Z$$

where

$$\langle \omega^p \rangle_Z \equiv \int_0^\infty \frac{d\omega}{\omega} \alpha^2 Z F(\omega) \omega^p \left/ \int_0^\infty \frac{d\omega}{\omega} \alpha^2 Z F(\omega) \right.$$ (26)

The results for $\langle \omega^p \rangle^{1/p}_Z$ with $p = 1$ and 2 at $T = 200$ K are given for both models in Table I. The moments $\langle \omega^p \rangle^{1/p}_{tr}$ of the transport spectral function $\alpha^2_{tr} F(\omega)$, from Eq.(11), that is, e.g.

$$\langle \omega^p \rangle^{1/p}_{tr} \equiv \int_0^\infty \frac{d\omega}{\omega} \alpha^2_{tr} F(\omega) \omega^p \left/ \int_0^\infty \frac{d\omega}{\omega} \alpha^2_{tr} F(\omega) \right.$$ (27)

are not listed in Table I, but are, in the RULN case, identical to the analogous moments of $\alpha^2 Z F$ and, in the MMP case, within 1% of the analogous $\alpha^2 Z F$ moments.

In conventional wide-band metals, with transport scattering dominated by phonons, we have $\lambda Z \sim 1$, $\Omega$ of the order of the Debye energy and hence $s$ of order $10^{-2}$. The Fermi-surface-restricted Boltzmann theory is thus expected to work quite well in such systems. However, in the MMP model, both $\alpha^2 Z F(\omega)$, from Eq.(23), and $\alpha^2_{tr} F(\omega)$, from Eq.(11), exhibit a wide peak, centered around $\omega_m \sim 90 - 120$ meV (depending on $T$), with substantial spectral weight extending up to the cut-off energy of $\Omega_c = 400$ meV, as shown for $T = 200$ K in Figs. 3a and 3b. With $\epsilon_F \sim 4 t_1 \sim 1.0$ eV (near $\frac{1}{2}$-filling), $\lambda Z \sim 1.6$ and $\Omega \sim 100 - 150$ meV (from Eq.(25) with $p \sim 1 - 2$), the Migdal parameter $s$ at 200 K is about $0.16 - 0.24$ here. Noticeable quantitative discrepancies between the full-zone Bethe-Salpeter and Fermi-surface-restricted Boltzmann theory can therefore be expected.

For the case of the RULN model, both $\alpha^2_{tr} F(\omega)$ and $\alpha^2 Z F(\omega)$, as shown in Figs. 3a and 3b, have a sharp peak around $\omega_m \sim 30 - 50$ meV and the spectral weight above $\omega_m$ decreases
more rapidly and is cut off altogether at $\Omega_c = 100$meV. This is reflected in a substantially smaller boson energy $\Omega \sim 30 - 50$meV, from Eq.(25) with $p \sim 1 - 2$. For the band and coupling parameters from column 2 of Table I, giving an Eliashberg parameter $\lambda_Z \sim 0.8$ and a Fermi energy $\epsilon_F \sim 4t_1 = 0.16$eV, the RULN model Migdal parameter at 200K, $s \sim 0.15 - 0.25$, is comparable to that of the MMP model.

However, if one chooses $t_1$ and $g^2$ in the RULN model so as to give the same bandwidth and the same resistivity as in MP-II, one finds the parameter estimates given in column 3 of Table I and discussed further below. For this parameter set, with $\epsilon_F \sim 4t_1 = 1.0$eV and $\lambda_Z \sim 1.3$, the Migdal parameter $s$ at 200K is only of the order $0.04 - 0.07$, i.e. noticeably smaller than in the MMP model. For this last RULN parameter set (column 3 of Table I), we therefore expect the Fermi-surface-restricted Boltzmann theory to provide a better approximation to a full-zone Bethe-Salpeter calculation of the resistivity.

The overall magnitude of the Migdal $s$ parameter in the MMP model raises serious concerns about the validity of the entire spin fluctuation exchange approach itself. It is well-known, that the validity of the Migdal-Eliashberg approximation rests on the smallness of that same parameter $s$, Eq.(24), which is also required to ensure the validity of the Fermi surface-restricted Boltzmann approach. In other words, the Migdal parameter $s$ which controls the relative magnitude of the discrepancy between full-zone Bethe-Salpeter and Boltzmann theory transport results, Fig. 2, also controls the relative magnitude of those higher-order non-Migdal vertex corrections which have been discarded, both in MP-II and in RULN, in the single-particle self-energy, in the particle-particle interaction kernel of the linearized Eliashberg $T_c$-equations, and in the particle-hole interaction kernel of the Bethe-Salpeter equation. One should therefore not be mislead into believing that numerical solutions of the full-zone Bethe-Salpeter equations necessarily constitute a "better" transport theory than the semi-classical Fermi-surface-restricted Boltzmann approach. Either approach works well when $s$ is sufficiently small compared to unity. And either approach can be expected to give, at best, only qualitatively correct results when the $s$ parameter attains magnitudes as large as estimated above. Concerns regarding the applicability of the Migdal approximation in spin fluctuation exchange models have already been raised in several earlier and recent studies.

IV. THE EFFECT OF SPECTRAL WEIGHT DISTRIBUTION ON $T_c$

The differences in the assumed band parameters and in the transport formalisms of RULN and MP-II certainly contribute to differences in their respective $d$-wave $T_c$ values. For the purpose of comparing the spin-fluctuation-mediated pairing in the two models, it is therefore of interest to treat the two models on an equal footing, as far as band parameters and transport formalism are concerned. In order to demonstrate that the differences in the $T_c$ values of the two models is not primarily caused by the differences in band parameters or transport formalism, we have thus carried out a $T_c$ calculation for the RULN model with the following modified parameter set, shown in column 3 of Table I:
Firstly, instead of \( t_1 = 40 \text{meV} \), we use the same LDA-based value \( t_1 = 250 \text{meV} \) which was assumed by MP. Secondly, with that \( t_1 \) value fixed, we adjust the RULN coupling constant \( g^2 \) so that the resistivity, calculated in both models at 200K in the Fermi-surface-restricted Kubo formalism, is the same, namely \( \rho = 109 \mu \Omega \text{cm} \). Recall that in the Fermi-surface-restricted Kubo formalism, Eqs.(8-12), the resistivity scales proportional to \( g^2/t_1^2 \), for fixed \( t \equiv t_2/t_1 \), band-filling and \( T \). Consequently, the modified \( g^2 \) value of 2.53eV\(^2\), thus obtained, in column 3, is about a factor of 9 larger than the \( g^2 \) estimate in column 2, in spite of the fact that the underlying \( \rho \) value is almost a factor of 4 smaller than that assumed in column 2.

The important point to notice now is that the resulting \( T_c \) = 18.4K for the modified RULN parameter values, in column 3, is increased only modestly over the original RULN estimate of 11.2K. Thus, in comparing the column 3 results for the RULN model to the MP-II results, in the last column of Table I, we conclude that the RULN \( T_c \) value is about a factor of 5 lower than the MP-II value, even if we assume the same model bandwidth, similar band-filling, and coupling constants \( g^2 \) giving similar values for the DC resistivity, calculated in both models, by the same transport formalism.

In fact, as noted earlier and clearly seen in Fig. 1, \( T_c \) as a function of \( g^2 \), in the RULN model, does not increase indefinitely with increasing \( g^2 \), but rather seems to approach a finite saturation value for \( g^2 \to \infty \). This saturation \( T_c \) does not exceed values of about 50K for the band parameters considered here. Using transport data and/or LDA bandstructure results to obtain actual estimates for \( g^2 \) and \( t_1 \) only serves to make this fundamental upper limit on \( T_c \) in the RULN model more stringent. Thus, given the RULN spin fluctuation spectrum of Eq.(4), with the spectral parameter values stated, it is simply not possible to generate, within a conventional Eliashberg theory, a \( d \)-wave \( T_c \) of, say, 90K or larger, regardless of the choice of band parameters and coupling strength \( g^2 \).

Why then does the RULN spin susceptibility give such a low \( T_c \), compared to the MMP model, even when its assumed bandwidth and resistivity is comparable to that of MP-II? To answer this, we define a pairing spectral function as follows

\[
\alpha_d^2 F(\omega) = -\frac{\pi a^2 \int \frac{d^2k}{(2\pi)^2} \int \frac{d^2k'}{(2\pi)^2} \delta(\epsilon_k)\delta(\epsilon_{k'})\eta(\vec{k})\eta(\vec{k}')\text{Im}V(\vec{k} - \vec{k}', \omega + i0^+)}{\pi \int \frac{d^2k}{(2\pi)^2} \delta(\epsilon_k)\eta^2(\vec{k})}
\]

where

\[
\eta(\vec{k}) = \cos(k_xa) - \cos(k_ya)
\]

is the basis function for nearest neighbor \( d_{x^2-y^2} \) pairing. Note here that the sign in Eq.(28) is defined such that a positive \( \alpha_d^2 F \) corresponds to attraction in the \( d \)-wave pairing channel. As shown in Fig. 3c, the spectral weight distribution of \( \alpha_d^2 F \) is quite similar to that of \( \alpha_z^2 F \) and \( \alpha_t^2 F \) in either model. Note here that, again, in the MMP model \( \alpha_d^2 F \) has a very broad peak, at an \( \omega_m \sim 35 - 55 \text{meV} \) (depending on \( T \)), with substantial spectral weight extending out to the 400meV cut-off. And, again, in the RULN model the spectral weight is much more narrowly peaked, at similar peak position \( \omega_m \sim 30 - 50 \text{meV} \), and falls off rapidly well before the 100meV cut-off. We emphasize that this latter spectral weight distribution is claimed to be in accord with the currently available neutron scattering data on \( \text{YBCO} \).
Recall now, from Eqs.(8-11), that the transport relaxation rate $1/\tau_0$, and hence the resistivity $\rho$, is most sensitive to the low-frequency part of $\alpha_{tr}^2 F$, up to $\omega \sim T$. Thus, with their $\omega_{p,0}$ values being about equal, the two models will give roughly the same resistivity if their respective coupling constants $g^2$ have been adjusted so that their $\alpha_{tr}^2 F$ are roughly the same, in absolute magnitude, at low frequencies $\omega \sim T$. However, given such coupling constant values, the MMP model will then give a much larger superconducting $T_c$ than the RULN model, because of its substantially larger spectral weight in $\alpha_{tr}^2 F$ at high frequencies.

The basic physical reason for this is that, unlike the normal state DC resistivity $\rho$, the superconducting transition temperature $T_c$ is quite sensitive to the high-frequency part of the boson spectrum.

To analyze this more quantitatively, we consider the moments and the dimensionless Eliashberg coupling parameters associated with $\alpha_{tr}^2 F$.

\[
\langle \omega^p \rangle_d = \int_0^{\infty} \frac{d\omega}{\omega} \alpha_d^2 F(\omega) \omega^p \right/ \int_0^{\infty} \frac{d\omega}{\omega} \alpha_d^2 F(\omega) \right. (30)
\]

and

\[
\lambda_d = 2 \int_0^{\infty} \frac{d\omega}{\omega} \alpha_d^2 F(\omega). (31)
\]

Notice that all frequency moments defined here and above ($\langle \omega^p \rangle_d^{1/p}, \langle \omega^p \rangle_{tr}^{1/p}$ and $\langle \omega^p \rangle_d^{1/p}$) are independent of the coupling strength $g^2$ and bandwidth $8t_1$, assuming fixed $T$, band shape $t \equiv t_2/t_1$ and band-filling. All the $\lambda$ parameters ($\lambda_Z, \lambda_{tr}, \lambda_d$), on the other hand, scale proportional to $g^2/t_1$, at fixed $T, t$ and filling.

In approximate $T_c$-formulas of the McMillan-Allen-Dynes variety, $T_c$ is given in terms of $\lambda_Z, \lambda_d$ and $\langle \omega^p \rangle_d^{1/p}$ by an expression of the form

\[
T_c \simeq \langle \omega^p \rangle_d^{1/p} F(\lambda_Z, \lambda_d) (32)
\]

where $p$ can be weakly $\lambda$-dependent with $0^+ \leq p \leq 2$. $F$ is monotonically increasing as a function of $\lambda_d$ and monotonically decreasing as a function of $\lambda_Z$. In the weak-coupling limit, $\lambda_d, \lambda_Z \ll 1$, $F$ varies roughly exponentially with $\lambda_Z$ and $1/\lambda_d$, that is

\[
F(\lambda_Z, \lambda_d) \simeq \text{const} \times \exp(-1/\lambda_d^*). (33)
\]

where

\[
\lambda_d^* = \frac{\lambda_d}{1 + \lambda_Z}. (34)
\]

Note however that, for the coupling strengths discussed here, in both models $\lambda_d, \lambda_Z \gg O(1)$, as shown in Table I. So both the MMP and the RULN model are really in a regime of intermediate, not weak, coupling. In this intermediate-coupling regime, the variation of $T_c$ with $\lambda_Z$ and $1/\lambda_d$ is typically less rapid than implied by Eq.(33).

The values of $\langle \omega \rangle_d, \langle \omega^2 \rangle_d^{1/2}, \lambda_d$ and $\lambda_d^*$, evaluated at the respective $d$-wave $T_c$’s, are shown in Table I. In comparing the RULN results, from e.g. column 3, to the MMP results, in the last column of Table I, there are three key points to be noted:
The first point is that the low-order frequency moments of $\alpha_2^2 F(\omega)$ in the MMP model are again significantly larger than those of the RULN model, by a factor of about 2-3. The second point is that also the pairing $\lambda$-parameter, $\lambda_d$, in the MMP model is about 2.2 times larger than the RULN value in column 3, despite the fact that both models have about the same $\lambda_{tr,0}$ at 200K. The third point is that, per $\lambda_d$, the MMP model has a noticeably smaller mass-enhancement $\lambda$-parameter, $\lambda_\text{tr}$, in the MMP model is about 0.88 in the MMP model, compared to 1.74 in the RULN model. The last two points imply that $\lambda_{tr}^*$ in the RULN model is noticeably smaller than in the MMP model.

In the McMillan-Allen-Dynes formalism, each of the foregoing three differences between the two models will tend to give the MMP model a larger $T_c$ than the RULN model. The first two differences, in $\langle \omega^p \rangle_d^{1/p}$ and $\lambda_d$, are an immediate consequence of the substantial additional high-frequency spectral weight in the MMP model, for $\omega > \sim 50$meV, as shown in Fig. 3c. The third difference, in the $\lambda_\text{tr}/\lambda_d$-ratio, is more subtle and arises from differences in the detailed momentum dependences of the two model susceptibilities.

To demonstrate more explicitly that the difference in the high-frequency spectral weight is indeed the primary cause for the differences in the $T_c$’s of the two models, we now consider what happens if we take, for example, the basic functional form of the RULN model, but allow it to have a substantially larger boson frequency scale than originally imposed by RULN on the basis of the neutron scattering data. That is, we modify the RULN spin susceptibility model by re-scaling its energy spectrum, leading to a modified susceptibility function

$$\chi_{\text{RULN},f}(\bar{q}, \omega) \equiv \chi_{\text{RULN}}(\bar{q}, \omega/f)$$

with a boson energy scaling factor $f$ and $\chi_{\text{RULN}}$ from Eq.(4). A re-scaled MMP model susceptibility $\chi_{\text{MMP},f}$ could be defined analogously with the MMP susceptibility $\chi_{\text{MMP}}$ from Eqs. (1) and (5). Notice here that all frequency moments, $\langle \omega^p \rangle_d^{1/p}$, $\langle \omega^p \rangle_{tr}^{1/p}$ and $\langle \omega^p \rangle_d^{1/p}$, scale linearly with $f$, whereas $\lambda_\text{tr}$ and $\lambda_d$ are independent of $f$, assuming $T$ and all other model parameters are fixed. From full-zone Eliashberg calculations, we find that, upon boson energy re-scaling at fixed $\lambda$ parameters, $T_c$ varies indeed roughly linearly with $\langle \omega^p \rangle_d^{1/p}$ in either model, consistent with the basic McMillan-Allen-Dynes approach, Eq.(32). Thus, by increasing the boson energy scale, with $f > 1$, at fixed $g^2$, we can raise the d-wave $T_c$ in the RULN model to values which are as large as those in the MMP model, or larger, while at the same time lowering the model’s normal state resistivity, above $T_c$, from Eqs.(8-12). Likewise, by lowering the overall boson energy scale, in either model, with $f < 1$, we would decrease $T_c$ and increase the resistivity $\rho$. Notice that $\lambda_{tr,0}$ and $\rho$, from Eqs. (8-12), decrease with increasing boson energy scale, since increasing $f$, at fixed $T$, actually reduces the relevant spectral weight of $\alpha_2^2 F(\omega)$ at low frequencies $\omega < \sim T$.

Suppose now we adjust both $g^2$ and $f$ in the re-scaled RULN model, Eq.(35), such that both its resistivity $\rho$ at $T = 200$K (from the the Fermi-surface-restricted Kubo formalism, Eqs. (8-12), say) and its d-wave $T_c$ (from full-zone Eliashberg solutions) match those of the MMP model, as given in the last column of Table I. The results for this last RULN parameter set are shown in column 4 of Table I. The required value for the scale factor is about $f = 2.70$, implying that, relative to column 3, all the various RULN frequency moments are increased by that factor. Also, the coupling constant $g^2$ and, hence all $\lambda$
values, are substantially increased, by more than a factor of 2, relative to those of column 3. This increase in $g^2$ is necessary in order to maintain a constant resistivity, $\rho = 109 \mu \Omega \text{cm}$, i.e. in order to compensate for the decreasing effect on $\rho$ caused by raising $f$.

In comparing the RULN results from column 4 to the MMP results in the last column of Table I, the crucial point to notice is that now both models, having the same $T_c$ and $\rho$, also have roughly, to within 20 – 30%, the same frequency moments. The fact that now the (re-scaled) RULN model acquires somewhat ($\sim 20 – 30\%$) larger frequency moments than the MMP model can be rationalized by noting that the smaller $\lambda_d^*$ in the RULN model has to be compensated for by a larger boson energy scale, in order to get the same $T_c$ as in the MMP model.

From the foregoing results, it is clear though that the spin fluctuation spectral weight distribution is the central factor determining $T_c$ in either model and that the differences in $T_c$ are not primarily caused by differences in bandstructure parameters or transport formalism.

V. SUMMARY

We can see now that the problem of whether high-$T_c$ superconductivity is explained by a spin fluctuation model is closely tied to the question about which type of dynamic susceptibility is more realistic, MMP or RULN. One important feature of the MMP model susceptibility is that its behavior is similar to an effective RPA form which is known to fit Monte Carlo data on the single band Hubbard model. That is, the peak in $\text{Im} \chi(q, \omega + i0^+)$ versus frequency is a strong function of momentum. In fact, the momentum dependence is so strong that it would imply the system to be very close to a magnetic instability, in contradiction to experiment. This problem is discussed further by Monthoux and Pines. By contrast, in the RULN model the $\omega$ peak position is independent of momentum. The latter behavior would seem unphysical from an effective RPA viewpoint, but is claimed to be consistent with presently available neutron scattering data on $YBCO$. On the other hand, it seems quite clear that substantial high frequency spectral weight is present in the undoped insulating cuprate parent compounds, since their AF magnon spectra must extend up to several hundred meV, assuming accepted estimates of the in-plane AF exchange constant $J \approx 100 \text{meV}$. It is therefore quite plausible that additional high-frequency spectral weight may also exist in heretofore unexplored energy regimes in the doped cuprates.

We thus feel that the crux of the matter lies in the neutron scattering data. The MMP form is based on NMR data which is essentially a zero-frequency measurement. We would argue that it is somewhat dangerous to infer the full frequency dependence of the susceptibility based on that data. There is hope that sufficiently reliable neutron scattering data, elucidating the complete momentum and frequency dependence, will become available to resolve these issues. We emphasize this since the significance and interpretation of current neutron scattering data has been a very controversial issue, especially in $YBCO$.

In this context the most recent neutron scattering data by Yamada et al. and by Hayden
et al. on La$_{2-x}$Sr$_x$CuO$_4$ (LSCO, with doping $x$ of 14 – 15%) are of considerable interest. These new data seem to imply that in the doped samples, the high-energy spectral weight (up to $\sim$ 300meV) in $\text{Im}\chi$ is substantially suppressed relative to the undoped, insulating antiferromagnetic parent ($x=0$) compound and that substantial low-energy spectral weight ($\sim$ 22meV) is being built up by doping. Also, the width in momentum space is relatively independent of frequency and implies a correlation length of order $a$. This observation would be quite consistent with an RULN picture. On the other hand, low frequency data show incommensurate peaks with a correlation length of 6.7 $a$. This rapid change of width in momentum space from low to high frequencies would be consistent with an MMP picture. It thus appears at this point that the new LSCO data are, in some sense, intermediate between the RULN and the MMP models. As Hayden et al. point out, their data are consistent with a broadened magnon dispersion, the functional form of which does not look like either model considered here.

On the theoretical side, we caution against over-interpreting the quantitative significance of results obtained from phenomenological spin fluctuation exchange models of the type discussed here. In order to produce a low resistivity and a high $T_c$, the typically required magnitude of the Migdal parameter $s$ in these models is sufficiently large to render the whole Migdal-Eliashberg approach invalid or, at the very least, makes it a rather questionable foundation for a quantitative theory. We also emphasize the often overlooked point that the conditions of applicability for the Fermi-surface-restricted Boltzmann transport theory are essentially the same as the conditions of validity for the Migdal approximation. Thus, as far as different transport formalisms are concerned, the Fermi-surface-restricted Boltzmann formalism is in principle “no worse” than the full-zone Bethe-Salpeter theory and, along with the Migdal approximation, either approach becomes quantitatively unreliable when the Migdal parameter $s$ is as large as we have found it for the spin fluctuation models considered here.

Finally, the required, rather large boson energy scales, with $\Omega/\epsilon_F \approx 0.1 – 0.2$, imply that extended (and, especially, nearest neighbor) Coulomb repulsions will substantially suppress the $d$-wave $T_c$ in the current AF spin fluctuation exchange models, since the conventional mechanism of reducing the effective Coulomb interaction strength via retardation becomes largely inoperative. Calculations based on current spin fluctuation models have so far neglected extended Coulomb interactions entirely and may thus seriously overestimate the maximum achievable $T_c$.

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Both the experimental data and calculated model results for \( \sigma(\omega) \) may already deviate noticeably from a simple Drude law, Eq.(7), for photon frequencies \( \omega > \frac{1}{\tau_D} \). To get at least a meaningful order-of-magnitude estimate for a "Drude" plasma frequency \( \omega_{p,D} \), we have thus parametrized the zero-frequency peak in \( \sigma(\omega) \) in terms of its peak height \( \sigma(0) \equiv 1/\rho \) and in terms of its peak width, \( 1/\tau_D \), defined here as the half-width at half-maximum (HWHM). We then use Eq.(13) as the defining relation for \( \omega_{p,D} \), that is

\[
\omega_{p,D} \equiv \left( \frac{4\pi}{\rho \tau_D} \right)^{1/2}.
\]

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In their original paper, RULN, Ref.[12], stated their coupling strength in terms of a dimensionless coupling parameter \( \bar{I}^2 \) which, in our present notation, is given by \( \bar{I}^2 = g^2 N_F C/\pi \) where \( N_F \) is the non-interacting density of states at the Fermi level. For a hole concentration \( n_h = 1.18 \) holes per planar Cu-site (i.e. a hole doping concentration of \( x = 18\% \)) and \( t \equiv t_2/t_1 = 0.45 \), we have \( N_F = 0.2481/t_1 \) and hence a conversion factor \( N_F C/\pi = 0.01500 eV^{-1}/t_1 \). Thus, for an assumed \( t_1 = 80 \) meV, the original upper limit value of \( \bar{I}^2 = 0.10 \), proposed by RULN, corresponds to a value of \( g^2 = 0.533 eV^2 \).

In RULN, Ref. [12], the transport relaxation time results where actually expressed in terms of the dimensionless transport \( \lambda \) parameter, \( \lambda_{tr,0} \equiv (2\pi T \tau_0)^{-1} \), from Eq.(10), which turns out to be approximately \( T \)-independent in the RULN model for \( T \gtrsim 200 K \). RULN adjusted their coupling strength \( g^2 \) (or \( \bar{I}^2 \), see previous footnote) so as to match the calculated \( \lambda_{tr,0} \) to the measured, approximately \( T \)-independent \( \lambda_{tr,D} \equiv (2\pi T \tau_D)^{-1} \). This procedure is of course entirely equivalent to adjusting \( g^2 \) so that \( \tau_0 \) becomes equal to \( \tau_D \).

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The quasi-particle mass enhancement due to spin fluctuations, \( Z_{sf} \), could be reduced, from the \( T = 0 \) estimate \( Z_{sf} \sim 1 + \lambda Z \), by thermal effects. In any boson exchange model of the types considered here, (including e.g. electron-phonon and spin fluctuation exchange systems), one can show that the relevant boson-exchange-generated mass enhancement factor \( Z \) (i.e. \( Z_{sf} \) in the present context) approaches unity when the temperature \( T \) becomes comparable to or larger than the characteristic boson energy scale \( \Omega \) [c.f., for example J. Zhong and H.-B. Schüttler (University of Georgia preprint, 1994)]. For the MMP model, \( \Omega \), as estimated e.g. by the low-order frequency moments of the spin fluctuation spectrum \( \alpha^2 F(\omega) \), Eq.(23) (see Table I), is of the order of 1000K and thus substantially larger than the relevant \( T \) range \( T \gtrsim 300 K \). However, for the RULN model, \( \Omega \) is only of order 300 – 400K and thermal effects could thus be noticeable in the \( T \)-range of interest here.

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TABLE I. Comparison of the RULN model, Eq.(4), and the MMP model, Eqs.(1) and (3). Abbreviations $FK$, $VB$, and $BS$ indicate transport results obtained at $T = 200K$ by the Fermi-surface-restricted Kubo and variational Boltzmann formalism, Eq.(10), and by solution of the full-zone Bethe-Salpeter equation, from Ref. [11], respectively.

| Model input parameters: | RULN | RULN | RULN | RULN | MMP |
|-------------------------|------|------|------|------|-----|
| $t_1$ [meV]             | 80   | 40   | 250  | 250  | 250 |
| $g^2$ [eV$^2$]          | 0.533| 0.267| 2.53 | 6.82 | 0.410|
| $f$                      | 1.00 | 1.00 | 1.00 | 2.70 | 1.00 |
| $N_L$                   | 1    | 2    | 2    | 2    | 2   |
| $n_h$                   | 1.18 | 1.18 | 1.18 | 1.18 | 1.25 |

$d$-Wave $T_c$ and transport:

| $T_c$ [K]                                     | RULN | RULN | RULN | RULN | MMP |
|-----------------------------------------------|------|------|------|------|-----|
| $\rho$ [$\mu\Omega$cm]                      | FK   | VB   | BS   |      |     |
|                                               | 447  | 556  |      |      |     |
|                                               | 109  | 150  |      |      | 132 |
| $\omega_{p,0}$ [eV]                          | FK   | VB   | BS   |      |     |
|                                               | 0.97 | 0.97 | 2.42 | 2.42 | 2.30|
| $\omega_{p,D}$ [eV]                          | BS   |      |      |      | 1.2 |
| $1/\tau_0$ [meV]                             | FK   | VB   | BS   |      |     |
|                                               | 57   | 71   |      |      |     |
|                                               | 86   | 107  |      |      | 94  |
|                                               | 86   | 107  |      |      | 94  |
| $1/\tau_D$ [meV]                             | BS   |      |      |      | 46  |
| $\lambda_{tr,0}$                              | FK   | VB   | BS   |      |     |
|                                               | 0.52 | 0.65 |      |      |     |
|                                               | 0.79 | 0.99 |      |      | 0.72|
|                                               | 0.79 | 0.99 |      |      | 0.72|
|                                               | 0.72 | 0.72 |      |      | 0.72|

Eliashberg $\lambda$ parameters:

| $\lambda_Z$ at $T_c$                       | RULN | RULN | RULN | RULN | MMP |
|---------------------------------------------|------|------|------|------|-----|
| $\lambda_d$ at $T_c$                       |      |      |      |      |     |
| $\lambda^*_d$ at $T_c$                     |      |      |      |      |     |

Frequency moments:

| $\langle \omega \rangle_Z$ [meV] at $T_c$ | RULN | RULN | RULN | RULN | MMP |
|-------------------------------------------|------|------|------|------|-----|
|                                            | 32.5 | 32.5 | 32.8 | 98   | 98  |
|                                            | 40.3 | 40.3 | 40.3 | 109  | 105 |
|                                            | 36.9 | 36.9 | 37.4 | 115  | 141 |
|                                            | 47.4 | 47.4 | 47.4 | 128  | 146 |
|                                            | 32.5 | 32.5 | 32.8 | 98   | 71  |
|                                            | 36.9 | 36.9 | 37.4 | 115  | 109 |

$\omega^2$ moments [meV]:

| $\langle \omega^2 \rangle_Z$ $^{1/2}$ [meV] at $T_c$ | RULN | RULN | RULN | RULN | MMP |
|------------------------------------------------------|------|------|------|------|-----|
| $\langle \omega^2 \rangle_d$ at $T_c$               |      |      |      |      |     |
| $\langle \omega^2 \rangle_d$ $^{1/2}$ [meV] at $T_c$ |      |      |      |      |     |
FIGURES

FIG. 1. $d$-wave superconducting transition temperature $T_c$ versus scaled coupling strength $\frac{g^2}{t_1}$ for the RULN model interaction potential $V(q,\omega) = g^2 \chi_{RULN}(q,\omega)$, Eqs.(4) and (5), with $t \equiv t_2/t_1 = 0.45$ and different values of $t_1$, as indicated in the figure. $T_c$ was calculated by full-zone solutions of the linearized Eliashberg equations on a $k$-mesh corresponding to $64 \times 64$ $k$-points covering the full 1st Brillouin zone, with fermion Matsubara frequencies $\nu_m \equiv (2m - 1)\pi T$ up to $m = 1024$, using FFT techniques, as described in Refs.[9-11,14-15].

FIG. 2. Resistivity $\rho$ versus temperature $T$ for the MMP model, obtained from the variational Boltzmann ($VB$, dot-dashed line) and from the Fermi-surface-restricted Kubo formalisms ($FK$, dashed line) Eqs.(8-12). For comparison, we also show the results of Monthoux and Pines, MP-II, Ref.[11], obtained from full-zone solutions of the Bethe-Salpeter transport equation ($BS$, full line) for identical model parameters, as given in the last column of Table I, with $T$-dependent $\omega_{sf}(T)$, $\chi_Q(T)$ and $\xi(T)$ given by Eq.(3).

FIG. 3. (a) $\alpha^2 tr F(\omega)$, Eq.(11), (b) $\alpha^2 Z F(\omega)$, Eq.(23), and (c) $\alpha^2 d F(\omega)$, Eq.(28), versus frequency $\omega$ for the MMP model, Eq.(1), and for the RULN model, Eq.(4), at different temperatures $T$. The RULN model parameters used are those from column 3 of Table I. The MMP model parameters used are those from the last column of Table I with $T$-dependent $\omega_{sf}(T)$, $\chi_Q(T)$ and $\xi(T)$ given by Eq.(3). The 3 different temperatures include the $d$-wave superconducting $T_c$ values of the RULN model, $T_{c,RULN} = 18.4$K, and of the MMP model, $T_{c,MMP} = 99.5$K, for the respective model parameters, as given in Table I, columns 3 and 5, respectively.
(b)\[\alpha^2 Z F(\omega)\]

0.0 \leq \alpha^2 Z F(\omega) \leq 1.0

\omega \text{ [meV]}

- 18.4K
- 99.5K
- 200.0K

RULN

MMP
