Quasi-Particle dynamics of a strongly correlated polaron metal

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Abstract
We develop a simple diagrammatic low-energy boson exchange strong-coupling model for an antiferromagnetically correlated polaronic metal. The model is based on a simplified, local anharmonic oscillator representation of the highly anharmonic Born-Oppenheimer lattice potential which typically arises in a finite density polaron system, as a result of polaronic self-localization. This Born-Oppenheimer potential exhibits a large manifold of nearly degenerate local potential minima, and hence a new class of low-energy excitations, associated with tunneling processes between the multiple Born-Oppenheimer wells. In the present paper, we employ a simple Migdal-type single-exchange diagrammatic approximation in order to study the what happens when conduction electrons are coupled to these anharmonic tunneling excitations via conventional electron-phonon interactions. Important low-temperature features of such a model are (i) a large polaronic mass enhancement $Z$ and a strongly narrowed, low-energy, near-Fermi-level van Hove resonance peak in the interacting density of states at temperatures $T$ well below the lattice tunneling energy scale $\Omega_t$; (ii) a rapid thermal suppression of $Z$ and of the van Hove resonance which occurs when the temperature $T$ becomes comparable to the lattice tunneling excitation energy scale $\Omega_t$; (iii) a broad incoherent background in the single-particle spectra $|G''(\vec{k},\omega)|$ near the Fermi energy; (iv) strongly flattened quasi-particle bands over wide regions of the Brillouin zone near the van Hove points; and (v) strong isotopic mass dependence of the ele-
Electronic mass enhancement $Z$ at temperatures $T$ well below $\Omega_t$ which, along with $Z$, becomes rapidly suppressed for $T$ comparable to $\Omega_t$.

Surprisingly, in spite of the large low-$T$ mass enhancement, the anharmonic lattice fluctuations in the high temperature regime $T \gtrsim \Omega_t$, give rise only to a moderate, essentially $T$-independent quasi-particle damping. This damping does not suppress coherent quasi-particle propagation in a wide, physically relevant parameter regime. We thus argue that, in a “weakly bound” finite-density polaron system, a novel polaron scenario may be realized where only the lattice motion, but not the quasi-particle propagation become incoherent in the high-$T$ regime. This scenario is in contrast to the conventional small-polaron strong-coupling picture, where the quasi-particle transport inevitably becomes incoherent at temperatures exceeding the polaron tunneling energy scale.

We also discuss possible implications of the anharmonic tunneling model for the cuprate superconductors. The predicted isotopic mass dependence of the low-$T$ ($T < \Omega_t$) electron quasi-particle mass enhancement provides a unique signature for the involvement of anharmonic tunneling fluctuations. We suggest possible low temperature isotope experiments to explore this question in the cuprates.

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I. INTRODUCTION

Hubbard-type strongly correlated electron models\textsuperscript{1} can adequately describe the low-lying charge and anti-ferromagnetic (AF) spin excitations in the undoped, insulating cuprate systems.\textsuperscript{2−5} However, in the doped systems, the low-energy physics may be substantially affected by coupling to the lattice degrees of freedom, since, \textit{in the presence of AF spin correlations}, already a rather weak electron-phonon coupling can cause polaronic self-localization of the dopant-induced charge carriers.\textsuperscript{6−10} As a consequence, large-amplitude anharmonic lattice displacement fluctuations occur, resulting from polaron tunneling motion.\textsuperscript{6−7} In the cuprate high-$T_c$ systems, there is indeed evidence for polaron formation and for large-amplitude, anharmonic lattice tunneling fluctuations of possible polaronic origin.\textsuperscript{11} However, the observed quasi-particle mass enhancements $Z \sim 2 - 4$ in the normal state of the doped, metallic cuprates\textsuperscript{12−19} fall far short of the magnitudes $Z \gtrsim 10 - 10^3$ (or larger) which one would naively expect to observe in a polaronic system.

In the present paper, we propose a new modeling approach towards the normal-state electron quasi-particle dynamics of an antiferromagnetically correlated polaronic metal where the essential features of the polaronic lattice dynamics\textsuperscript{6−7} and AF spin fluctuation exchange\textsuperscript{20−29} are combined into a generalized Migdal-type diagrammatic treatment. The polaronic lattice anharmonicity does then indeed lead to large polaronic mass enhancement $Z$ when the temperature $T$ and excitation energies $\omega$ are well below a certain, generally small lattice tunneling energy scale $\Omega_t$.

However, for $T \gtrsim \Omega_t$, the polaronic contribution to $Z$ is suppressed and $Z$ is dominated by the smaller spin fluctuation contribution. The polaronic lattice fluctuations contribute then only to the quasi-particle damping, in a manner quite similar to – and experimentally indistinguishable from – disorder scattering. Surprisingly, in spite of the large low-$T$ mass enhancement, the high-$T$ quasi-particle damping caused by the anharmonic lattice fluctuations is quite modest and the
electronic transport dynamics retains essentially coherently propagative character. This suggests the possibility of a heretofore unexplored “weakly bound” polaron scenario wherein polaron formation does not inevitably lead to complete incoherence at temperatures exceeding the polaron tunneling energy scale. Our treatment thus suggests a novel approach towards dense polaron systems which bridges the gap between the conventional Fermi-liquid-based Migdal theory of delocalized, harmonic electron-phonon systems and the strong-coupling methods developed originally for the strongly localized, single-electron small-polaron problem.

The remainder of the paper is organized as follows: In Section II, we outline the basic underlying ideas of polaronic anharmonicity in the lattice dynamics of a strongly correlated electron-phonon system; we propose a simple exactly numerically solvable model for the polaronic Born-Oppenheimer potential; and we discuss the effective electron-electron interaction $V_{AP}$ which is mediated by exchange of the anharmonic tunneling excitations arising from the lattice quantum dynamics within such an “anharmonic phonon” potential. We then combine this lattice-mediated electron interaction $V_{AP}$ with a simple electron-electron model interaction $V_{SF}$ describing AF spin fluctuation exchange. The full model interaction $V = V_{AP} + V_{SF}$ then serves as our input into a self-consistent diagrammatic single-electron self-energy calculation, which we formulate at the level of a Migdal-type single-exchange approximation for a single-band conduction electron system on a two-dimensional (2D) square lattice. From the self-energy, we extract important physical quantities such as the electron quasi-particle dispersion $E_{\vec{k}}$, and and the quasi-particle mass enhancement $Z$, the single-electron spectral function $G''(\vec{k},\omega)$ and the the momentum-integrated density of states $\rho(\omega)$.

In Section III, we discuss basic physical principles governing the polaronic mass enhancement in our diagrammatic model. We show, by analytical arguments, how, within our diagrammatic model, one can recover, at least qualitatively, the central results for polaronic mass enhancement which are conventionally derived within a non-perturbative electron-phonon strong-coupling theory. Important im-
plications for a potential observable isotopic mass dependence in the electron mass enhancement are discussed in the anharmonic tunneling exchange model and contrasted with a corresponding harmonic phonon exchange model. Based on self-consistent numerical self-energy calculations, we then discuss the temperature ($T$-) dependence of the polaronic self-energy and its implications for the $T$-dependence of the quasi-particle mass enhancement $Z$ and of the quasi-particle damping. We then consider the effects of anharmonic tunneling fluctuation exchange on the momentum integrated density of states and, in particular on the van Hove singularity. Numerical results for the single-particle spectral functions and for the overall quasi-particle band dispersion in the full Brillouin zone will also be discussed.

Lastly, in Section IV, we present a summary of our results, with emphasis on potential experimental implications of our model calculations for the cuprate high $T_c$ materials. We conclude with an outline of the generic features of our model which are likely to be of general physical significance and likely to be recovered in a more realistic polaron model.

II. LATTICE TUNNELING FLUCTUATION EXCHANGE MODEL

A. Polaronic anharmonicity

As a simplest model, we start from a two-dimensional (2D) antiferromagnetically correlated Hubbard-type single-band electron system on a 2D square lattice,\textsuperscript{1−5,20−29} coupled to an Einstein optical phonon system via a Holstein electron-phonon interaction\textsuperscript{6−10,32−37}

$$H_{EP} = \sum_j C u_j (n_j - 1).$$  \hspace{1cm} (1)

Here, $C$ denotes the deformation potential coupling constant, $n_j = 0, 1, 2$ the electron occupation, and $u_j$ the local Einstein oscillator displacement at lattice sites.
Physically, $u_j$ could represent, for example, a collective coordinate for local breathing-type displacements of planar or apical oxygens in the cuprates.

In the absence of EP coupling, the lattice dynamics is governed by a bare harmonic restoring potential $W_P(\{u_j\})$ corresponding to a non-interacting phonon Hamiltonian

$$H_P = \sum_j \frac{1}{2M}p_j^2 + W_P(\{u_j\})$$

where $M$ is the atomic or molecular mass associated with each displacement degree of freedom $u_j$ and $p_j \equiv -i\hbar \partial/\partial u_j$ is the conjugate momentum of $u_j$. In the simplest microscopic strongly correlated electron-phonon model, the Holstein-Hubbard model\textsuperscript{6,7,9,32–37} $W_P$ is given by an Einstein potential

$$W_P(\{u_j\}) = \sum_j \frac{1}{2}Ku_j^2$$

with a bare, harmonic restoring force constant $K$. To be specific, we will, for the following discussion, adopt the Holstein-Hubbard model as our underlying microscopic model Hamiltonian. The basic ideas are more general, however, and can, in principle, be extended to more complicated electron-phonon systems exhibiting polaronic self-localization. The EP coupling strength can then be quantified by a characteristic energy

$$E_P = \frac{C^2}{K}$$

which measures the strength of the phonon-mediated on-site attraction, as well as the single-polaron binding energy in the ionic (zero-bandwidth limit) of the Holstein-Hubbard model.

In the nearly $\frac{1}{2}$-filled Holstein-Hubbard electron system with sufficient EP coupling strength $E_P$, a dopant-induced carrier of, e. g., hole-type, $n_j = 0$, self-localizes.\textsuperscript{6–9} That is, by locally distorting the lattice by some $\Delta u_j \equiv d_t$, the carrier creates an attractive electron potential well, of depth

$$\Delta_P \equiv Cd_t$$
and thus lowers its energy by forming a bound state.\cite{6,7,32,37} The inter-site tunneling motion of such polaronic carriers causes the displacement $u_j$ at each site $j$ to fluctuate between two distinct equilibrium positions, $u_\pm$, with $|u_+ - u_-| \simeq d_t$.

As explained at length in Refs. [6,7,38], this physical picture can be fully captured within the framework of the Born-Oppenheimer approximation, that is, in terms of a renormalized lattice potential $W(\{u_j\})$.\cite{6,7,38} In the full microscopic treatment, based on the Holstein-Hubbard model,\cite{6,7} this Born-Oppenheimer potential is given by the total ground state energy of the 0th order adiabatic Hamiltonian $H_{ad}(\{u_j\})$ which depends parametrically on the fixed, $c$-number lattice displacements $\{u_j\}$. $H_{ad}(\{u_j\})$ consists of the bare potential $W_P(\{u_j\})$, the EP coupling term $H_E(\{u_j\})$ and the purely electronic part $H_E$ which is independent of the displacements $u_j$. In the case of the Holstein-Hubbard model, $H_E$ is just the standard Hubbard Hamiltonian.\cite{1,2,3,4,5} Detailed microscopic studies along these lines, based on analytical considerations and on numerical many-body total energy calculations on finite clusters have been carried out.\cite{6,7,9}

These microscopic studies reveal that the transition or cross-over from the delocalized carrier regime to the self-localized carrier regime is fundamentally accompanied by a qualitative change in the character of the renormalized lattice potential $W$. In the delocalized carrier regime, the low-energy lattice dynamics is governed essentially by one lowest, absolute potential minimum in $W(\{u_j\})$. Quadratic expansion of $W(\{u_j\})$ around its minimum, thus leads again to an essentially harmonic lattice dynamics where the primary renormalization effect of the EP coupling is to modify the harmonic restoring force constants, relative to $W_P(\{u_j\})$.

In the self-localized carrier regime, on the other hand, $W(\{u_j\})$ acquires a highly degenerate, anharmonic, multiple-minimum low-energy structure wherein different local minima of $W$ correspond to different possible real-space configurations of the self-localized carriers. The polaron tunneling dynamics in this Born-Oppenheimer picture can then be described in terms of lattice tunneling
processes between “adjacent” $W$-minima. The low-energy structure of the Born-Oppenheimer energy surface is thus highly complex, especially, at a finite polaron density, involving, in general highly anharmonic, highly non-local multi-site interactions between the $u_j$ coordinates. The low-energy lattice tunneling dynamics within this degenerate multi-well structure is further complicated by the presence of non-trivial $e^{i\pi}$ Berry phase factors which arise from adiabatic electron ground-state wavefunction overlaps during the adiabatic tunneling motion of the lattice between different local $W$-wells.\(^7\) Trying to calculate, or even simulate, the low-energy lattice dynamics in the self-localized regime, from a “realistic”, that is, microscopically based Born-Oppenheimer potential does not appear to be feasible at the present time, especially in the physically most interesting case of finite polaron carrier densities.

We are therefore proposing to simplify the polaronic lattice dynamics problem by replacing the microscopic lattice potential with a drastically simplified model potential. This simplified potential does not, by any measure, capture all the intricate details of the microscopic potential. Nevertheless, as we will show, it retains some of the essential physical features of the polaronic lattice dynamics. Furthermore, this model potential can serve as the starting point for more realistic modeling approaches which may capture some of those physical aspects, such as non-local multi-site anharmonicity, which our present model fails to include.

Specifically, we propose to model the polaronic lattice potential by the following ansatz

$$W(\{u_j\}) = \sum_j w(u_j) \equiv \sum_j \Delta_B[2(u_j/d_t)^4 - (u_j/d_t)^2] . \quad (6)$$

The single-site potential $w(u_j)$ is a local (on-site) double-well with minima at

$$u_{\pm} = \pm d_t/2 . \quad (7)$$

The two potential minima in $w(u_j)$ are separated by a tunneling barrier of height $\Delta_B$ and width $d_t$. 

- 8 -
Eq. (6) captures some of the essential physics of the polaronic lattice dynamics, namely, the fact that each \( u_j \) undergoes large-amplitude fluctuations between two distinct equilibrium positions \( u_\pm \). Neglected in this simple model potential are all the anharmonic inter-site correlations described above within the microscopic framework.\(^6\,^7\)

The essential new feature of the polaronic lattice dynamics, which is absent in harmonic phonon systems, is a new class of large-amplitude, low-energy inter-well tunneling excitations, which exist in addition to the familiar, small-amplitude, intra-well phonon-like excitations. In our model, Eq. (6), these two types of excitations are represented by the excitation energies \( \Omega_t \) and \( \Omega'_h \) of, respectively, the 1st and 2nd excited state, measured from the groundstate, in the single-site double-well \( w(u) \). For reasonable parameters, we find

\[
\Omega_t \ll \Omega'_h \tag{8}
\]

where \( \Omega'_h \) is comparable to the single-well harmonic phonon energy which can be estimated by

\[
\Omega_h \equiv \hbar \left( \frac{K_h}{M} \right)^{1/2} \tag{9}
\]

where the single-well harmonic restoring force

\[
K_h \equiv \frac{\partial^2}{\partial u^2} w(u_\pm) = 40 \frac{\Delta_B}{d_i^2} \tag{10}
\]

is determined by the curvature of the potential at the single-well minimum and \( M \) is the atomic/molecular mass associated with the local oscillator degree of freedom \( u \). In a full microscopic Holstein-Hubbard calculation,\(^6\) \( \Omega_h \) is generally comparable to the bare \( (C \equiv 0) \) harmonic phonon energy \( \Omega_{h0} = \hbar (K/M)^{1/2} \).

**B. Fluctuation exchange potentials**

By exchange of anharmonic lattice excitations an effective electron-electron interaction \( V_{AP} \) is mediated.\(^{39-43}\) As in standard harmonic phonon exchange
models, this anharmonic phonon exchange potential $V_{AP}(\vec{q}, i\omega)$ can be expressed as a product of electron-lattice coupling constants [i.e $C^2$ in our model, Eq. (1)] and appropriate lattice displacement correlation functions. That is, in our model, following Refs. [39-43],

$$V_{AP}(\vec{q}, i\omega) = -C^2 \int_0^\beta d\tau \frac{1}{N} \sum_{j,\ell} e^{i\omega\tau - i\vec{q} \cdot (\vec{r}_j - \vec{r}_\ell)} \langle u_j(\tau)_{AP} u_\ell(0) \rangle_{AP} .$$

(11)

for an electron-electron momentum-energy transfer $(\vec{q}, i\omega)$ where $i\omega \equiv 2n_\omega \pi T$ is the even Matsubara frequency with integer $n_\omega$. $N$ denotes the number of lattice sites on an $N = L \times L$ 2D square lattice lattice with periodic boundary conditions, $\vec{r}_j$ and $\vec{r}_\ell$ are the position vectors of lattice sites $j$ and $\ell$, respectively, $\beta \equiv 1/T$ is the inverse temperature. The notations $\langle ... \rangle_{AP}$ and $u_j(\tau)_{AP}$ in Eq.(11) indicate thermal averaging and, respectively, evolution in imaginary time $\tau$, according to a Born-Oppenheimer effective lattice Hamiltonian given by

$$H_{AP} = \sum_j \frac{1}{2M} p_j^2 + W(\{u_j\}) \equiv \sum_j h_{u_j} .$$

(12)

For our simple local model potential, Eq. (6), $H_{AP}$ describes $N$ uncoupled local double-well oscillator degrees of freedom $u_j$, each subject to the local Hamiltonian

$$h_u = \frac{1}{2M} p^2 + w(u) ,$$

(13)

which acts only on a single local degree of freedom $u$.

Because the simple on-site coupling, Eq. (1), and local model potential, Eq. (6), $V_{AP} \equiv V_{AP}(i\omega)$ becomes $\vec{q}$-independent in our model, and can be expressed in terms of the local (single-site) eigenstates of $h_u$. Namely, written in terms of its spectral representation,

$$V_{AP}(i\omega) = \int_{-\infty}^{+\infty} \frac{d\omega'}{\pi} \frac{V_{AP}'(\omega')}{\omega' - i\omega} .$$

(14)

where the spectral function on the real-$\omega'$ axis, $V_{AP}''(\omega') \equiv \frac{1}{2}[V_{AP}(\omega' + i0^+) - V_{AP}(\omega' - i0^+)]$, is given by

$$V_{AP}''(\omega') = -\pi \sum_{\iota,\kappa} |\langle \psi_\kappa | u | \psi_\iota \rangle|^2 \frac{e^{-\beta\eta_\kappa}}{z_h} [\delta(\eta_\kappa - \eta_\iota - \omega') - \delta(\eta_\kappa - \eta_\iota + \omega')] .$$

(15)
Here, \( \psi_\iota(u) \) denotes the normalized eigenstates of \( h_u \) with eigenenergy \( \eta_\iota \), labeled in ascending order, beginning with the groundstate \( \iota \equiv 0 \). Also, \( z_h \equiv \sum_\iota \exp(-\beta \eta_\iota) \) is the corresponding single-site partition function. \( V''_{AP} \) can thus be easily evaluated by solving numerically the single-site Schrödinger equation for \( h_u \), to obtain \( \psi_\iota \) and \( \eta_\iota \). By carrying out the \( \iota \)- and \( \kappa \)- summation in Eq. (15) numerically up to, say, the 5-th excited state, \( \iota, \kappa \leq 5 \), one captures over 99\% of the total spectral weight in \( V''_{AP} \), assuming physical parameter values given below.

We augment \( V_{AP} \) by a simple model for the electron-electron interaction potential, \( V_{SF}(\vec{q},i\omega) \), mediated by the AF spin fluctuations.\(^\text{20–29} \) The model potential is defined for the 2D square lattice \textit{via} its spectral spectral representation

\[
V_{SF}(\vec{q},i\omega) = \int_{-\infty}^{+\infty} d\omega' \frac{V''_{SF}(\vec{q},\omega')}{\omega' - i\omega} \quad (16)
\]

with a spectral function\(^\text{44} \) of the form\(^\text{24} \)

\[
V''_{SF}(\vec{q},\omega) = -g_s^2 \sum_{\vec{Q}^*} F(\vec{q} - \vec{Q}^*) \Phi''(\omega) . \quad (17)
\]

A simple continuous, \( \vec{q} \)-independent linear spin fluctuation spectrum is assumed, with\(^\text{24} \)

\[
\Phi''(\omega) = \frac{2\omega}{\Omega_s^2} \Theta(\Omega_s - |\omega|) . \quad (18)
\]

extending up to a typical spin fluctuation cutoff \( \Omega_s \). The \( \vec{q} \)-dependence is assumed to be Lorentzian\(^\text{24} \)

\[
F(\vec{q} - \vec{Q}^*) = \frac{A_{SF}}{|\vec{q} - \vec{Q}^*|^2 + \kappa_{AF}^2} \quad (19)
\]

with a half-width \( \kappa_{AF} \) of order of the inverse AF correlation length. The \( \vec{Q}^* \) summation in Eq. (17) is over the four equivalent AF wavevectors

\[
\vec{Q}^* = (\pi, \pi), (-\pi, \pi), (-\pi, \pi), (-\pi, -\pi) . \quad (20)
\]

The overall normalization factor \( A_{SF} \) is chosen so that

\[
g_s^2 = \frac{-1}{N} \sum_\vec{q} \int_0^\infty d\omega V''_{SF}(\vec{q},\omega) \quad (21)
\]
where $g_s^2$ is the spin fluctuation coupling constant and the $\vec{q}$-summation is only over the 1st Brillouin zone of the 2D square lattice with lattice constant $a$. Also, Eq. (17) is understood to apply only to $\vec{q}$-points within the 1st Brillouin zone, with periodic continuation beyond the 1st zone boundaries.

We should emphasize here again that the foregoing simplified model potentials can reproduce only the most qualitative physical features of the order of magnitude, of the $T$-variation and of the $\omega$-dependences of various physical quantities discussed below. For instance, no $T$-dependence is built into the spin fluctuation exchange potential. Likewise, the spectral and thermal properties of the polaronic lattice dynamics has been severely simplified here, to retain physical features such as large-amplitude tunneling fluctuations and a low tunneling ($\Omega_t$) energy scale, while neglecting, e.g., all effects from inter-site lattice couplings which, surely, will alter the details of the $T$- and $\omega$-dependence of $V''_{AP}$. Therefore, these potentials cannot and should not be expected to reproduce, say, details of the quasi-particle spectral shapes or of the $T$-dependence of quasi-particle lifetimes.

C. Self-energy calculation

From the total interaction $V \equiv V_{AP} + V_{SF}$, we obtain the single-electron self-energy $\Sigma$ in a self-consistent Migdal single-exchange approximation.\textsuperscript{30,31,44} In the Matsubara frequency domain, this single-exchange diagram for the single-electron self-energy is given by\textsuperscript{30,31,44}

\begin{equation}
\Sigma(\vec{k}, i\nu) = -\frac{T}{N} \sum_{\vec{k}', i\nu'} V(\vec{k} - \vec{k}', i\nu - i\nu') G(\vec{k}', i\nu')
\end{equation}

where $\vec{k}$ and $\vec{k}'$ denote electron momenta and $i\nu \equiv (2n_{\nu} + 1)\pi T$ and $\nu'(2n'_{\nu} + 1)\pi T$ are odd Matsubara frequencies with integer $n_{\nu}$ and $n'_{\nu}$.

The fully dressed electron Green’s function in Eq. (22) is given by the Dyson equation

\begin{equation}
G(\vec{k}, i\nu) = \frac{1}{i\nu - \epsilon_{\vec{k}} - \Sigma(\vec{k}, i\nu)}
\end{equation}
where $\epsilon_{\vec{k}}$ is the non-interacting single-electron conduction band structure. We are adopting a single-band tight-binding model with 1st neighbor hybridization $t$ only, again defined on the 2D square lattice appropriate to a single $CuO_2$ layer in the cuprates. Hence, for $\vec{k} \equiv (k_x, k_y)$,

$$\epsilon_{\vec{k}} = -2t[\cos(ak_x) + \cos(ak_y)] - \mu$$

(24)

with the chemical potential $\mu$ absorbed in $\epsilon_{\vec{k}}$.

The basic idea underlying this diagrammatic approach is that, at the level of the Born-Oppenheimer approximation, all renormalizations of the phonon system due to EP coupling are, in principle, contained in the effective lattice potential $W$. Hence, the displacement correlation function in Eq. (11) represents, in principle, the fully dressed phonon propagator and $V_{AP}$ must, in this context, be regarded as the already fully screened phonon-mediated electron-electron interaction potential, which can be directly inserted into the Migdal single-exchange diagram, without further renormalization. Beyond the well-controlled Born-Oppenheimer approximation, there are thus two primary further approximations being made here: firstly, the replacement of the quite complex polaronic multiple-well lattice potential by the simple local double-well model, Eq. (6), and, secondly, the neglect of higher-order vertex corrections, in the Migdal approximation. Of these two, the former is likely to be the more severe one; the latter can actually be roughly justified for the model parameter values employed below, based on standard order of magnitude estimates for the leading order vertex correction. Another essential – and likely uncontrolled – approximation is of course the treatment of AF spin fluctuation exchange within the Migdal approximation. This constitutes a common, fundamental problem in all presently existing diagrammatic AF spin fluctuation exchange theories. We have, in that regard, no further progress to offer in the present paper.

By standard analytical continuation techniques, Eq. (23) can be recast into the real-frequency domain to yield the self-energy spectral function $\Sigma''$ on the
real-ω axis, expressed in terms of the spectral functions of \( V \) and \( G \), namely

\[
\Sigma''(\vec{k}, \omega) \equiv \frac{1}{2} [\Sigma(\vec{k}, \omega + i0^+) - \Sigma(\vec{k}, \omega - i0^+)]
\]

\[
= \frac{1}{N} \sum_{\vec{k}'} \int_{-\infty}^{+\infty} \frac{d\omega'}{\pi} V''(\vec{k} - \vec{k}', \omega - \omega') G''(\vec{k}', \omega') \times [b(\omega - \omega') + 1 - f(\omega')].
\]  

(25)

Here, \( f(\omega) \equiv 1/(e^{\beta\omega} + 1) \) and \( b(\omega) \equiv 1/(e^{\beta\omega} - 1) \) denote the Fermi and Bose factor, respectively, and the \( \vec{k}' \)-integral is over the 1st Brillouin zone of the 2D square lattice. The spectrum of the single-electron Green’s function in Eq. (25) is given by

\[
G''(\vec{k}, \omega) \equiv \frac{1}{2} [G(\vec{k}, \omega + i0^+) - G(\vec{k}, \omega - i0^+)]
\]

\[
= \frac{\Sigma''(\vec{k}, \omega)}{[\omega - \epsilon_{\vec{k}} - \Sigma'(\vec{k}, \omega)]^2 + [\Sigma''(\vec{k}, \omega) + 0+]^2}
\]

(26)

and \( \Sigma' \) is obtained from the self-energy spectral function \( \Sigma'' \), via the Kramers-Kronig relation

\[
\Sigma'(\vec{k}, \omega) \equiv \frac{1}{2} [\Sigma'(\vec{k}, \omega + i0^+) + \Sigma'(\vec{k}, \omega - i0^+)] = \oint \frac{d\omega'}{\pi} \frac{\Sigma''(\vec{k}, \omega')}{\omega' - \omega}
\]

(27)

where \( \oint \) denotes the principal value integral.

Eqs. (25)-(27) are solved iteratively, starting from the 0-th order ansatz for the self-energy \( \Sigma_0 \equiv 0 \). To evaluate \( \Sigma'' \) for \( N \to \infty \) numerically in the real-frequency domain, Eq. (25), with high \( \omega \)-resolution, we use a modified, 2D adaptation of the so-called “tetrahedron method”\(^{46}\) to carry out the \( \vec{k}' \)-integral in Eq. (25). Specifically, to handle the \( \vec{k}' \) integration over the nearly singular quasi-particle peak structure of \( G'' \) efficiently, the inverse of the electron Green’s, from Eq. (23), that is \( 1/G(\vec{k}, \omega \pm i0^+) \) [not \( G(\vec{k}, \omega \pm i0^+) \)] and, separately, the \( \vec{q} \)-dependent factor of the interaction potential, \( V'' \), from Eqs. (17),(18), are linearly interpolated over small triangular \( \vec{k} \)-elements. Upon, expressing \( G'' \equiv \text{Im}G \) in terms of the \( G \), so interpolated, the \( \vec{k}' \)-integral over each such triangular element can be calculated.
To construct the triangular interpolation grid, the Brillouin zone is covered with an \( N = L \times L \) grid of equal square elements where each square is then subdivided along a diagonal into two equal triangles. To preserve the 4-fold point symmetry of the lattice in the resulting triangular grid, the subdividing diagonal is chosen to be along the \((+1, +1)\)-direction for square elements in the 1st and 3rd quadrant \([ i. e. \{ \vec{k} = (k_x, k_y) \mid k_xk_y > 0 \}]\), and along the \((+1, -1)\)-direction for square elements in the 2nd and 4th quadrant \([ i. e. \{ \vec{k} = (k_x, k_y) \mid k_xk_y < 0 \}]\) of the Brillouin zone. The numerical results shown below were obtained on grids with \(2N = 2 \times 40 \times 40\) and \(2N = 2 \times 80 \times 80\) triangular elements. Comparisons between the two grid sizes at a few selected parameter values, including \(T = 0\), indicate general agreement of the self-energy results at the \(1 - 2\%\)-level or better.

The chemical potential \(\mu\) is adjusted so that the electron concentration

\[
\langle n_j \rangle = -\frac{2}{N} \sum_{\vec{k}} \int_{-\infty}^{+\infty} f(\omega) G''(\vec{k}, \omega)
\]

equals the specified input value. Note that the prefactor 2 arises from summation over the electron spin and \(f(\omega) \equiv 1/(e^{\beta\omega} + 1)\) denotes again the Fermi factor.

The self-consistent quasi-particle band \(E_{\vec{k}}\) is then obtained from the solution of

\[
E_{\vec{k}} = \epsilon_{\vec{k}} + \Sigma'(k, E_{\vec{k}}).
\]

The interacting Fermi surface is defined as the locus of all \(\vec{k}\)-points \(\vec{k}_F\) where

\[
E_{\vec{k}_F} = 0.
\]

The mass enhancement factor on the Fermi surface is

\[
Z(\vec{k}_F) \approx 1 - \partial_\omega \Sigma'(\vec{k}_F, \omega = 0).
\]

Corrections to \(Z\) due to \(\partial_\vec{k} \Sigma'\) are \(\lesssim 5 - 15\%\), for the parameters studied, and henceforth neglected.
III. RESULTS AND DISCUSSION

A. Selfenergy and mass enhancement

Before discussing the numerical results obtained with the above described method, we will first try to obtain a qualitative analytical understanding of the self-energy and mass enhancement results obtained at low excitation energies and temperatures $|\omega|, T \ll \Omega_t$.

For $T \ll \Omega_t$, the mass enhancement $Z$ is dominated by the low-energy ($\sim \Omega_t$) lattice tunneling excitations. To estimate this, let us first consider the tunneling contribution to the potential, $V_t$, in Eq. (15). By isolating the low-$T$ tunneling term, that is, the contribution arising from the excitation $\iota=0 \rightarrow \kappa=1$ from the ground- to the 1st excited state, we get

$$V''_t(\omega) = -\pi |\langle \psi_1|u|\psi_0 \rangle|^2 [\delta(\Omega_t - \omega) - \delta(\Omega_t + \omega)] , \tag{32}$$

using $\Omega_t \equiv \eta_1 - \eta_0$ and the fact that the Boltzmann weight filters out the ground-state in Eq. (15) at $T \ll \Omega_t$, i. e., $\frac{1}{z_h} \exp(-\beta \eta_0) \approx \delta_{t,0}$.

To estimate the transition matrix element in Eq. (32) we introduce the “single-well” basis states

$$\psi_{\pm}(u) \equiv \frac{1}{\sqrt{2}} [\psi_1(u) \pm \psi_2(u)] . \tag{33}$$

Assume that the overall phase of both $\psi_0(u)$ and $\psi_1(u)$ has been chosen such that they are both real-valued and both positive for $u \sim u_+$, that is both $\psi_{\pm}(u)$ have positive amplitude in the “right” well of their double well potential $w(u)$. Clearly then $\psi_+(u)$ must be localized with most of its probability weight in the “right” well of $w(u)$, near $u = u_+$, and likewise, by parity, $\psi_-(u) = \psi_+(u)$ in the “left” well, near $u = u_-$. At sufficiently high tunneling barrier, i. e. roughly when $\Omega_t \ll \Omega'_h \equiv \eta_2 - \eta_0$, the spatial overlap between $\psi_+$ and $\psi_-$ in either well becomes negligibly small with $|\psi_+(u)|^2$ and $|\psi_-(u)|^2$ sharply peaked near $u_+$ and,
respectively, near \( u_- \). We can thus estimate their \( u \)-matrix elements by a simple tight-binding-like approximation, namely

\[
\langle \psi_\sigma | u | \psi'_\sigma \rangle \cong u_\sigma \delta_{\sigma, \sigma'}
\]

for \( \sigma, \sigma' \in \{+, -\} \), hence

\[
\langle \psi_1 | u | \psi_0 \rangle = u_+ = d_t/2.
\]  

(35)

Inserting the foregoing \( \langle \psi_1 | u | \psi_0 \rangle \) into Eq. (32) and the resulting \( V_t \) into Eq. (25), we can now calculate the tunneling contribution to \( \Sigma'' \). This is greatly simplified by the fact that \( V_t \) is \( \vec{q} \)-independent, \( i. e. \), the \( \vec{k}' \)-integral can be rewritten as a frequency integral over the interacting electron density of states

\[
\rho(\omega) \equiv \frac{1}{N} \sum_{\vec{k}} \frac{1}{\pi} \Pi(-) G''(\vec{k}, \omega).
\]  

(36)

In the limit \( T \to 0 \) and \( |\omega| \gtrsim \Omega_t \ll \Omega'_t \), we get

\[
\Sigma''(\omega) \cong -\frac{\pi}{2} \Gamma_t \Theta(\Omega_t - |\omega|)
\]

where

\[
\Gamma_t = \frac{1}{2} \rho(0) C^2 d_t^2.
\]

(38)

The gap-like depletion of spectral weight in Eq. (37), \( i. e. \) the fact that \( \Sigma''(\omega) = 0 \) for electronic single-particle energies \( |\omega| \) up to \( \Omega_t \) simply reflects the threshold behavior associated with the density of states of the tunneling excitations: At \( T = 0 \), an electron or hole quasi-particle with an excitation energy \( |\omega| \), measured from the Fermi level, cannot loose more than \( |\omega| \) in an inelastic emission or scattering process. Hence the electron or hole cannot undergo any such inelastic processes if \( |\omega| \) falls below \( \Omega_t \), which is the lowest bosonic excitation energy available for emission into the lattice system. Also, at \( T = 0 \), there are no thermal lattice excitations present to be absorbed by the quasi-particle. Hence the damping \( |\Sigma''| \) vanishes for \( |\omega| < \Omega_t \).
Inserting Eq. (37) into the Kramers-Kronig relation (27), we find $\Sigma'_t$ and, from that, the tunneling contribution to the mass enhancement

$$Z_t \equiv -\partial_\omega \Sigma'_t(0) \cong \frac{\Gamma_t}{\Omega_t}. \quad (39)$$

Since $\Gamma_t$ is comparable to electronic energies, whereas $\Omega_t$ is small compared even to typical phonon energies $\Omega'_h$, we get $Z_t \gg 1$. In fact, in our model, Eq. (6), we have very roughly

$$\Omega_t \sim \Omega_h \exp(-c_t \Delta_B / \Omega_h) \quad (40)$$

with $c_t$ of order unity. From microscopic calculations of $W$, we also know that $\Delta_B \sim E_P$ in the EP strong-coupling limit.\(^6\),\(^7\) Combining these results, we thus recover quite naturally in our diagrammatic approach the central result from strong-coupling-limit polaron theory, namely\(^6\),\(^7\),\(^33\) that the electron mass enhancement increases exponentially with $E_P / \Omega_h$, that is

$$Z_t \sim \frac{\Gamma_t}{\Omega_h} \exp(c_t E_P / \Omega_h). \quad (41)$$

The foregoing results, Eq. (40),(41), apply primarily in the strongly anharmonic limit $\Delta_B \gg \Omega_h$. However, even in the intermediate regime $\Delta_B \sim \Omega_h$, $\Omega_t$ and hence $Z_t$ will still remain sensitively dependent on $\Delta_B$, and, via $\Omega_h$ [Eqs (9),(10)], on $M$ and $d_t$.

In the present diagrammatic model, the $T = 0$ mass enhancement is thus caused directly by the narrow, gap-like depletion in the self-energy spectrum discussed above. The detailed spectral shape of $\Sigma''$ is of course model-dependent. However, the gap-like spectral weight depletion, over a very narrow energy range $\sim \Omega_t$ around the Fermi level, and the overall electronic magnitude of $|\Sigma''| \sim \Gamma_t \gg \Omega_t$ are generic features of the lattice-mediated interaction $V_{AP}$ in the presence of polaronic anharmonicity. Via the Kramers-Kronig relation, Eq. (27), these features of $\Sigma''$ are directly translated into the large $Z$ seen in $\Sigma'$.

Another important feature of the tunneling mass enhancement $Z_t$ is its strong dependence on the isotope mass $M$ of the lattice degrees of freedom. To see this,
note first that, all lattice-related model parameters such as \( \Delta_B, d_t \) and \( C \) and all bandstructure and spin fluctuation-related model parameters, such as \( t, g_s, \kappa_{AF}, \Omega_s \) and \( \mu \) must be regarded as being of purely electronic origin. That is, in the general Born-Oppenheimer framework, all these parameters do not depend sensitively on \( M \). As a consequence, the damping strength \( \Gamma_t \), from Eq. (38), is also \( M \)-independent. However, \( \Omega_h \propto M^{-1/2} \), as given by Eq. (9), does depend on \( M \). In contrast to this rather modest power-law \( M \) dependence of \( \Omega_h \), the tunneling splitting \( \Omega_t \) is rather sensitive to changes in \( M \). The “exponential” \( M \)-dependence of \( \Omega_t \), reflected roughly in Eq. (40), holds only in the strongly anharmonic limit where \( \Delta_B > \Omega_h \) and \( \Omega_t \ll \Omega_h \). However, \( \Omega_t \) will retain a substantial \( M \)-dependence even at weaker anharmonicity where \( \Delta_B \sim \Omega_h \gtrsim \Omega_t \). Hence, a strong isotopic mass dependence of \( Z_t \) arises in our model, via Eq. (39), from the fact that the damping strength \( \Gamma_t \) is independent of \( M \), whereas \( \Omega_t \) is sensitively dependent on \( M \).

It is of interest to compare the foregoing results from the anharmonic tunneling model to conventional harmonic phonon exchange. To make this comparison meaningful, we specifically ask what happens if we replace the anharmonic double-well \( w(u) \), Eq. (6), by a “corresponding” single-well potential

\[
w_h(u) = \frac{1}{2} K_h u^2
\]

whose the harmonic restoring force constant \( K_h \) is chosen to coincide with the curvature of the double-well minima in \( w(u) \), i.e., \( K_h = 40\Delta_B/d_t^2 \) as given by Eq. (10) and the corresponding harmonic phonon frequency \( \Omega_h = \hbar (K_h/M)^{1/2} \) by Eq. (9). We also assume the same EP coupling constant \( C \).

The derivation of the self-energy contribution \( \Sigma_h \) and mass enhancement contribution from this harmonic Einstein phonon exchange model is standard. The self-energy spectrum \( \Sigma''_h \) has the same analytical form as \( \Sigma''_t \) in Eq. (37), with \( \Omega_t \) replaced by \( \Omega_h \) and \( \Gamma_t \) replaced by a \( \Gamma_h \), given analogous to Eq. (38) by

\[
\Gamma_h = \frac{1}{2} \rho(0) C^2 d_h^2 \equiv \rho(0) \frac{C^2}{K_h} \Omega_h
\]
Here the anharmonic tunneling fluctuation amplitude $d_t$ in Eq. (38) has been replaced by $d_h \equiv (2\Omega_h/\hbar K_h)^{1/2}$ which represents, in physical terms, the harmonic oscillator zero-point fluctuation amplitude. An important point to note here is that, again, $d_t$ in the double-well model is entirely a property of the Born-Oppenheimer potential function $w(u)$, and hence purely electronic in origin, i.e. it does not depend on the isotopic mass $M$. By contrast, $d_h$, and hence $\Gamma_h$ do depend on $M$.

Analogous to Eq. (39), the harmonic phonon exchange contribution to the self-energy is estimated by

$$Z_h \equiv -\partial_\omega \Sigma_h'(0) \equiv \Gamma_h/\Omega_h = \rho(0)\frac{C^2}{K} \equiv \lambda_h$$

which is of course just the conventional dimensionless Eliashberg EP coupling parameter $\lambda_h$, written down here for the simple case of a harmonic Einstein model. Comparing Eq. (44) to Eq. (41), we thus find that replacing the harmonic Einstein oscillator well $w_h(u)$ by the double well $w(u)$ increases the lattice contribution to the electron mass enhancement by a factor

$$\frac{Z_t}{Z_h} = \frac{d_t^2}{d_h^2} \frac{\Omega_h}{\Omega_t}$$

which will be large compared to unity, if the double well is wide, $d_t \gg d_h$, and/or the tunneling excitation energy is small, $\Omega_t \ll \Omega_h$.

An essential difference between the harmonic phonon and the anharmonic tunneling exchange model is their respective isotopic mass dependence which, in $Z_t$, is strong whereas, in $Z_h$, is absent, since $\Omega_h$ cancels out in Eq. (44). The predicted isotope dependence of $Z_t$ can therefore be used as a crucial experimental test to establish or refute the participation of large-amplitude lattice tunneling excitations in the low-energy electronic properties of the cuprates. Angle-resolved photoemission spectroscopy (ARPES) measurements of the electron quasi-particle dispersion, the electronic specific heat, the Drude weight in the low-frequency optical conductivity and, in the superconducting state, the low-temperature ($T \ll T_c$)
London penetration depth are possible candidates for exploring the isotopic mass
dependence of the electron mass enhancement in the cuprates. Some experimental
data for the isotopic mass dependence of the penetration depth in one cuprate
material already exist\(^47\) and appear to indeed show a strong isotope dependence
of \(Z\). However, we caution that these data\(^47\) are rather limited, have not been re-
produced independently at the present time, and their interpretation is presently
still controversial.\(^48\)

Indirect evidence for a strong isotope effect in \(Z\) can be inferred from the
extensively studied isotopic mass dependence of the superconducting transition
temperature \(T_c\) in the cuprates,\(^49,50\) quantified in terms of the isotope exponent
\(\alpha \equiv -\partial \log(T_c)/\partial \log(M)\) In several non-optimally doped cuprates systems, values
of \(\alpha\) in the range \(0.2 - 1.0\) are routinely observed, even in samples having \(T_c\)-values
as large as \(40 - 60K\).\(^49,50\)

In theoretical studies of purely electronic AF spin fluctuation exchange pairing
models, giving rise to a \(d_{x^2-y^2}\)-pairing instability, one finds\(^51\) that the inclusion of
harmonic phonon exchange suppresses \(T_c\) primarily via the phononic contribution
\(Z_h\) to the electron mass enhancement. As a consequence, the phononic \(T_c\) sup-
pression is largely independent of the isotope mass, due to the absence of isotopic
mass dependence in \(Z_h\), and the isotope exponent is small, typically \(|\alpha| < 0.05\),
in harmonic phonon models. Large \(|\alpha|\) values, \(|\alpha| \sim 0.5 - 1.0\), could be produced
by harmonic phonon exchange only if the EP coupling in the model was made so
strong that \(T_c\) is suppressed to unrealistically low values (\(< 10K\)). By contrast,
in spin fluctuation exchange \(d\)-wave pairing models with anharmonic tunneling
exchange, of the type described in the present paper, large values of \(\alpha\), of order
1.0 and larger, could be easily reproduced without substantial suppression of \(T_c\).\(^51\)
Taken in conjunction with the experimental isotope data,\(^49,50\) the model calcula-
tions suggests, that the isotopic mass dependence of lattice contribution to \(Z\) is
indeed much stronger than coupling to a harmonic phonon system would allow to
produce.
The foregoing conclusions\textsuperscript{51} apply to any electronic “excitation exchange” pairing model, with added coupling to harmonic phonon or, respectively, anharmonic lattice tunneling degrees of freedom, and they go well beyond the specific framework of the AF spin fluctuation exchange mechanism. We caution however that the model isotope calculations\textsuperscript{51} are fundamentally based on the assumption that the pairing is primarily of electronic origin and that it can be described within this general perturbative framework of an electronic “boson exchange” theory. The latter assumption is by no means firmly established and or accepted at the present time. More detailed experimental studies of the possible isotopic mass dependence in the low-energy electronic excitation spectrum of the cuprates would therefore be exceedingly helpful in establishing or refuting the participation of anharmonic tunneling fluctuations in these materials.

In interpreting such isotope experiments, especially in the normal state of the cuprates, it will be important to recognize that the predicted strong isotopic mass dependence of $Z$ is limited to the low-temperature regime. This is illustrated by Fig. 1 which shows numerical results for the $T$-dependence of $Z$, obtained from Eq. (31), and also, separately, the anharmonic tunneling contribution to $Z$, denoted by $Z_{AP}$, both calculated at the Fermi wavevector $\vec{k}_F$ along the $(1,1)$-direction, where

$$Z_{AP}(\vec{k}_F) \equiv -\partial_{\omega} \Sigma_{AP}(\vec{k}_F, 0) \quad (46)$$

and $\Sigma_{AP}$ is the contribution to $\Sigma$ due to $V_{AP}$ in Eqs. (22),(25). The calculation was done with a set of model parameters which is representative for the cuprates, namely $\langle n_j \rangle = 0.75$, that is a hole doping concentration of $x \equiv 1 - \langle n_j \rangle = 25\%$, $t = 0.35eV$,\textsuperscript{2} and spin fluctuation parameters\textsuperscript{24} $g_s = 1.06eV$, $\Omega_s = 0.105eV$ and $1/\kappa_{AF} = 3.33a$ with a lattice constant $a = 3.8\AA$. Also,\textsuperscript{6} $C = 3.27eV/\AA$, $\Delta_B = 75.29meV$, $d_t = 0.257\AA$, and $M = 16u$ for the lattice atomic mass, so that\textsuperscript{6,11} $\Omega_t = 10meV$, $\Omega'_h = 50meV$ and $\Omega_h = 97.3meV$.

For $T \ll \Omega_t$, we find numerically that $V_{AP}$, $\Sigma_{AP}$ and $Z_{AP}$ are indeed dominated by the low-energy tunneling excitation $i = 0 \rightarrow \kappa = 1$ [Eq. (15)] in $V_{AP}$.
Hence, $V_{AP}$, $\Sigma_{AP}$ and $Z_{AP}$ are essentially the same as, respectively, the $V_t$, $\Sigma_t$ and $Z_t$ discussed above. Our analytical estimate $Z_t = \Gamma_t/\Omega_t$, with $\Gamma_t$ from Eq. (38) and the density of states $\rho(\omega = 0, T = 0) \approx 0.175 t^{-1}$ from the inset of Fig. 2, gives $Z_t \approx 17.6$. This must be regarded as reasonable order-of-magnitude agreement with the numerical $T = 0$ result $Z_{AP} \approx 8.75$ in Fig. 1. The analytical overestimate, by about a factor of 2, is due to the fact that our estimate for the tunneling matrix element $|\langle \psi_1 | u | \psi_0 \rangle| \approx d_t/2$, entering into $\Gamma_t$, is an overestimate. Eq (34) is strictly valid only in the large-barrier limit $\Delta_B \gg \Omega_h$ which is not well realized here. Another factor affecting the quantitative accuracy of our analytical estimates for $\Sigma''$ and $Z_t$ is the assumption of an approximately constant $\rho(\omega)$, on $\omega$-scales of order $\Omega_t$. In the vicinity of the van Hove singularity [see Fig. 2 inset and discussion below], this becomes a somewhat crude approximation.

Along other directions of the Fermi wavevector, we find numerically quite similar results. The overall dependence of $Z$ and $Z_{AP}$ on the direction of $\vec{k}_F$ is weak. For example, for $\vec{k}_F$ along the $(1,0)$-direction, $Z$ is about $10\%-20\%$ larger than in the $(1,1)$ direction, with quite similar $T$-dependence.

The important point to notice in Fig. 1 is that, while $Z_{AP}$ accounts for about 60% of the total $Z$ at low $T$, $Z_{AP}$ is rapidly suppressed when $T$ becomes comparable to the tunneling energy scale $\Omega_t$. This happens because, upon raising $T$, the low-energy spectral gap in $\Sigma''_{AP}$, Eq. (37), gets "filled in," since thermally excited quasi-particles can now emit and absorb thermal tunneling excitations and thus cause damping, that is $|\Sigma''| > 0$ even at $\omega = 0$.\textsuperscript{30,31,44} Already for $T \sim \Omega_t$, most of the $2\Omega_t$-gap in $\Sigma''$ and, along with it, most of the polaronic mass enhancement $Z_{AP}$ has disappeared.

Above this characteristic "mass suppression" temperature scale, $T \gtrsim \Omega_t$, $V_{AP}$ contributes only a $T$- and $\omega$-independent damping to $\Sigma''$ which is physically quite similar to disorder scattering. The mass enhancement $Z$ is then dominated by the spin fluctuation contribution $V_{SF}$. In fact, as indicated by the dashed line in Fig. 1, for $T \gtrsim 2\Omega_t$, the mass enhancement in the full "anharmonic phonon + spin
The "fluctuation" (APSF) model becomes indistinguishable from that of the pure spin fluctuation (SF) model (without $V_{AP}$). This $T$-independent damping contribution can also be estimated analytically for $T \gg \Omega_t$. The result is roughly

$$\Sigma''_{AP}(\omega) \approx -\frac{\pi}{2} \Gamma_t \sim \text{const} \quad (47)$$

for all $\omega \ll t$. Note that this is the same value as found for low $T$ at $\omega$ above the excitation threshold, $\omega > \Omega_t$ in Eq. (37). Note also that this damping contribution is independent of the isotope mass $M$, as discussed above.

The foregoing high-$T$ results in the anharmonic phonon model should also be contrasted with the conventional harmonic phonon exchange model. In the latter, the mass enhancement contribution $Z_h$ becomes thermally suppressed when $T \sim \Omega_h$. However, the $T$-dependence of the electron quasi-particle damping contribution $|\Sigma''_h|$ is quite different in the high-$T$ region, since $|\Sigma''_h| \sim \lambda_h T$ rises linearly with $T$. This difference in the $T$-dependence is generic to the two types lattice dynamics models. These different $T$-dependences arise because in the harmonic model at $T > \Omega_h$, the amplitude square of the fluctuating EP potential seen by the electrons, $C^2\langle u_j^2 \rangle$, increases linearly with $T$, by the equipartition theorem. By contrast, in the anharmonic tunneling model, this amplitude square has a much weaker $T$-dependence, since $C^2\langle u_j^2 \rangle \sim C^2d_t^2/4$ is determined, at both low and high $T$, primarily by fluctuations between two wells, not by fluctuations within a single well.

For comparison, we also quote the approximate, Fermi surface averaged analytical results for the spin fluctuation contributions to the self-energy, $\Sigma_{SF}$, and to the mass enhancement, $Z_{SF}$. Using standard Fermi surface averaging procedures, we obtain from Eqs. (17)-(19) and (25) for temperatures $T \ll \Omega_s$,

$$\Sigma''_{SF}(\omega) = -\frac{\pi}{4} \Gamma_s \min \left[ \frac{\omega^2}{\Omega_s^2}, 1 \right] \quad (48)$$

and

$$Z_{SF} = \frac{\Gamma_s}{\Omega_s} \quad (49)$$
where
\[
\Gamma_s = \frac{16}{\pi} \rho(0) g_s^2 \langle F \rangle_{FS}
\]  
(50)
and the Fermi surface average of \( F(\vec{k} - \vec{k}' - \vec{Q}^*) \) from Eq. (19), denoted by \( \langle F \rangle_{FS} \), is of order unity. The low-energy spectral weight depletion in \( \Sigma''_{SF}(\omega) \) extends to \( \Omega_s \). At excitation energies \( \omega \) on the order of the tunneling energy scale \( \Omega_t \), with \( \Omega_t \ll \Omega_s \), the spin fluctuation contribution to the damping is
\[
|\Sigma''_{SF}(\Omega_t)| = \frac{\pi}{4} \Gamma_s (\Omega_t/\Omega_s)^2 = \frac{\pi}{4} \frac{Z_{SF}}{Z_{AP}} \frac{\Omega_t}{\Omega_s} \Gamma_t \ll \Gamma_t .
\]  
(51)
This is small compared to the lattice tunneling contribution \( |\Sigma''_{AP}(\Omega_t + 0^+)| = (\pi/2)\Gamma_t \), even though the respective mass enhancement contributions \( Z_{SF} \) and \( Z_{AP} \) may be of comparable magnitude.

At very high temperatures, comparable to the spin fluctuation energy scale \( \Omega_s \), \( Z_{SF} \) will be suppressed by the thermal excitation mechanism in the spin fluctuation system, analogous to the thermal suppression of \( Z_{AP} \) described above. Because of the much higher energy scale \( \Omega_s \), the onset of the thermal suppression of \( Z_{SF} \) is much more gradual, but it can already be clearly seen in the (compared to \( \Omega_s \)) relatively low temperature regime \( T \lesssim 0.2t \) shown in Fig. 1. Given their large \( \Omega_s \) scale, this \( Z_{SF} \) suppression effect may not be very important in the cuprates, up to, say, 1000K.

**B. Coherent vs. incoherent polaron dynamics**

In spite of the large low-\( T \) mass enhancement \( Z_{AP} \), the anharmonic lattice contribution to the damping in the high-\( T \) regime is quite modest, of order \( |\Sigma''_{AP}| \approx (\pi/2)\Gamma_t \sim 0.28eV \), using the parameter set from Fig. 1 and Eq. (38). Assuming a high-\( T \) value \( Z \sim 4 \), say [see Fig. 1], this translates into an anharmonic tunneling contribution to the quasi-particle decay and transport relaxation rates of order
\[
\frac{1}{\tau_{AP}} \approx \frac{|\Sigma''_{AP}|}{Z} \sim 70\text{meV} .
\]  
(52)
This is roughly the right order of magnitude magnitude, compared to typical single-particle and Drude peak widths measured in the normal state of the cuprates in the 200 – 400K range.\textsuperscript{12–19,53} Recall here that the quasi-particle decay rates and transport relaxation rates, as reflected in the single-particle and Drude spectral (HWHM) peak widths, \textit{are} being renormalized by the $1/Z$-factor, along with the quasi-particle dispersion $E_k$.

It is frequently argued that polarons cannot exhibit coherent transport at temperatures exceeding some very low “de-coherence” energy scale, set roughly by the single polaron bandwidth, of order $8t/Z_P$ in our 2D model, as estimated in the single-polaron strong-coupling theory.\textsuperscript{33,34} Here, the strong-coupling polaron band width renormalization $Z_P$ can be easily as large as $10 – 10^4$ (or larger) and is exponentially dependent on the EP coupling strength and atomic mass, roughly as given in Eq. (41). According to this \textit{single-polaron, strong-coupling} picture, polarons are inevitably condemned to incoherent propagation, by hopping-type transport mechanisms,\textsuperscript{33} when $T$ becomes comparable to $8t/Z_P$. Our foregoing diagrammatic results suggest otherwise:

The above estimated high-$T$ decay time, from Eq. (52), and the resulting mean free path, are still about an order of magnitude away from the Mott-Ioffe-Regel limit, \textit{i. e.} well on the coherent side of that limit. The quasi-particles, albeit damped, remain coherent at high-$T$, due to the fact that the polaronic mass enhancement $Z_{AP}$ is being suppressed at $T \gtrsim \Omega_t$ and due to the fact that the high-temperature “remnants” of the low-$T$ anharmonic tunneling fluctuations do not scatter the quasi-particles very strongly. At least for the specific parameter set used above, the scattering from the “remnant” anharmonic fluctuations is by no means sufficient to drive the electron quasi-particles into the incoherent / hopping type regime. The physical picture that emerges here is that, at $T \gtrsim \Omega_t$, only the coherence of the lattice tunneling groundstate – but not the coherence of the electronic quasi-particles – is being lost when $T$ reaches the \textit{lattice} tunneling energy scale.
How can these two seemingly quite contradictory physical pictures be reconciled? The answer, we believe, lies in the parameters. The above-described strong-coupling small polaron picture is based on the EP strong-coupling limit where, in the underlying microscopic EP model, the EP coupling strength $E_P \equiv C^2/K$ exceeds the bare bandwidth $8t$ and, at the same time, the tunneling barrier heights $\Delta_B$ of the polaronic Born-Oppenheimer lattice potential $W$ and the polaron binding energies (relative to the delocalized carrier state) are large, namely, of order $E_P$.

In this limit the polaronic lattice fluctuation amplitude $d_t$ is of the order$^{6,7}$ $d_t \sim C/K$, hence $Cd_t \sim E_P$, and in our local double-well lattice model, Eq. (6), the condition $E_P \gg t$, via Eq (38), translates into

$$\Gamma_t \sim \frac{1}{2} \rho(0)E_P^2 \sim \frac{E_P}{8t}E_P \gg t.$$  \hspace{1cm} (53)

We are assuming here $\rho(0) \sim 1/8t$ so that $\rho(0)E_P \sim O(1)$. Under these conditions, our diagrammatic approach breaks down at $T \sim \Omega_t$, but, nevertheless, the diagrammatics signals its own inadequacy, as the quasi-particle damping, estimated from Eq. (47), will indeed approach or exceed the Mott-Ioffe-Regel limit.

This strong-coupling picture is inevitably correct for low-density polaron systems with a nearly empty conduction band and with short-range EP coupling in spatial dimensions $D \geq 2$. In this type of EP system, the conditions $\Delta_B \sim E_P \gg t$ must be satisfied in the polaronic regime because, unless $E_P > E_P^{(\text{crit})} \gg t$, polarons will simply not be formed.$^{35}$ Here, $E_P^{(\text{crit})}$ denotes the minimum EP coupling strength needed to stabilize the polaronic self-localized carrier state against delocalization. In the nearly empty-band situation, $E_P^{(\text{crit})}$ is of order of the bandwidth or larger.$^{6,35}$

However, in the case of the Holstein-Hubbard (and related) models, as applied to the cuprates, polaron formation arises in the near $1/2$-filled band limit and the polaronic carriers are dopant induced holes in a strongly correlated Mott-Hubbard insulator electron background. Extensive microscopic calculations$^{6-9}$ have shown
that the presence of AF spin correlations in the near 1/2-filled Hubbard electron system drastically reduces the threshold for polaron formation in such a system, roughly to $E_P^{(\text{crit})} \sim 2 - 3t$ in realistic parameter regimes. Furthermore, for $E_P$ near $E_P^{(\text{crit})}$, the lattice potential barriers separating different polaronic minima can become quite small, so that $\Delta_B \ll t$ or even $\Delta_B \sim \Omega_h$ and also $C d_t < E_P$. In this limit, we get

$$\Gamma_t < \frac{1}{2} \rho(0) E_P^2 \lesssim t$$

In this “weakly bound polaron” regime, a diagrammatic treatment based on a coherent quasi-particle picture is likely to become applicable, even for $T \gtrsim \Omega_t$. On the other hand, the strong-coupling expansion, based on the assumption $E_P \gg t$, is likely to fail here.

It is conceivable that microscopic EP models may exhibit a cross-over from the strongly bound regime, Eq. (53), to the weakly bound regime as a function of increasing doping and/or increasing temperature. Such a cross-over can be driven by mutual screening of the attractive polaronic EP potential wells. This screening occurs at finite polaron density when nearby polaronic self-localized wavefunctions and EP potential wells begin to overlap. It has the effect of lowering the height $\Delta_B$ and the width $d_t$ of the polaronic inter-site tunneling barriers in the lattice potential $W$. This barrier screening effect has recently been demonstrated by microscopic calculations for the Holstein-Hubbard model.\(^7\) Thermal de-trapping of the polaronic carrier from its EP potential well will also tend to enhance this barrier screening effect by increasing the population of unbound carriers. Hence, raising the temperature can have qualitatively the same effect as raising the doping level, namely, to push the system towards weaker polaronic binding energies and lower barrier heights. It will be interesting to investigate whether such a cross-over is realized in at least some of the cuprates which, as a function of doping and temperature seem to show evidence of hopping-type conductivity at low doping and low $T$, but exhibit apparently coherent transport at larger doping and/or higher $T$. 

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\(^7\) This is a reference to a previous study or work.
The partially ionic character of the cuprates and resulting spatially extended Fröhlich-type EP couplings are another factor which may contribute to the existence of a “weakly bound” polaron regime. Such long-range EP couplings have the effect of lowering the overall threshold $E_P^{\text{crit}}$ by allowing “large” (i.e. spatially extended) polaron formation to occur even in dimension $D \geq 2$.\textsuperscript{35,54} Extensive phenomenological studies have so far considered only large bi-polarons and only in the context of continuum models.\textsuperscript{35,54} It will be of considerable interest to investigate such longer-range EP coupling with discrete crystal lattice models and to explore the cross-over from large / weakly bound to strong-coupling / strongly bound polaron behavior.

C. Density of states and single-electron spectra

In Fig. 2, we show the resulting density of states, $\rho(\omega)$, calculated for the same parameter set as in Fig. 1, from Eq. (36), at $T = 0$ and at $T = 0.029t \cong \Omega_t$. The most prominent feature in Fig. 2 is the narrow, strongly $T$-dependent peak in close proximity to the Fermi level $\omega \equiv 0$ in $\rho(\omega)$, as shown by the full line in Fig. 2.\textsuperscript{55} At $T = 0$, we can show that $\rho(\omega)$ near the Fermi level is essentially just a narrowed image of the non-interacting density of states\textsuperscript{44} $\rho^{(0)}(\omega)$ for the same band filling, that is, for $|\omega| \sim \Omega_t$

$$\rho(\omega) \cong \rho^{(0)}(\bar{Z}\omega)$$

with $\bar{Z}$ denoting the $\vec{k}_F$-average of $Z$. The “resonance” peak in Fig. 2 is thus primarily a narrowed image of the non-interacting 2D van Hove singularity and its peak position $\omega_{vHs}$ relative to the Fermi level $\omega = 0$ is roughly given by

$$\omega_{vHs} = \frac{\omega_{vHs}^{(0)}}{\bar{Z}}$$

where $\omega_{vHs}^{(0)}$ denotes the position of the van Hove singularity, relative to the Fermi level, in the corresponding non-interacting system at the same band filling.
A rough derivation of this result, Eq. (55), can be sketched as follows: First, neglect the $\vec{k}$ dependence of $\Sigma$ around the Fermi surface and replace $\Sigma(\vec{k},\omega)$ by an appropriate Fermi surface average $\bar{\Sigma}(\omega)$. Second, neglect the small imaginary part $\bar{\Sigma}''$ and approximate its real part by the standard “Fermi liquid” approximation

$$\bar{\Sigma}'(\omega) \approx (1 - \bar{Z})\omega + O(\omega^2)$$

(57)

where $\bar{Z} \equiv 1 - \partial_{\omega}\bar{\Sigma}(0)$. Third, insert this into Eqs. (26) and the resulting $G''$ into Eq. (36) to arrive at Eq. (55).

Note, in Fig. 2, that the logarithmic divergence at the van Hove singularity has been slightly smeared out, even at $T = 0$, by the damping ($|\Sigma''| > 0$) at finite $\omega$ and by the $\vec{k}$ dependence of $\Sigma$ along different directions on the Fermi surface. These damping and $\vec{k}$-dependence effects are neglected in the derivation of Eq. (55). Also, as shown in the inset of Fig. 2, the resonance peak is rapidly suppressed, along with $Z(T)$, when $T$ becomes comparable to $\Omega_t$. This is again caused by the strong thermal damping at $\omega = 0$ and by the thermal suppression of $Z(T)$, when $T$ becomes of order $\Omega_t$ or larger. Because of the thermal damping effects, the density of states peak in the “APSF” model (including $V_{AP}$) is suppressed faster with increasing temperature than in the pure “SF” model (without $V_{AP}$, see dashed line in Fig. 2 and inset); the APSF model generates an additional strong damping already when $T \sim \Omega_t$ which is absent in the SF model.

A careful study of the doping dependence of the density of states peak near $\omega = 0$ reveals that, while substantially contributing to this peak, the van Hove singularity in the non-interacting density of states $\rho^{(0)}$ is not necessarily required to generate such a $\rho(\omega)$-peak. Even for a completely flat $\rho^{(0)}(\omega)$, e. g. at band fillings where the van Hove singularity is far away from Fermi level $\omega = 0$, it is possible to obtain a pronounced peak structure in $\rho(\omega)$ near the Fermi level. The general conditions under which this happens are that the self-energy spectrum $|\Sigma''(\vec{k}_F,\omega)|$ on the Fermi surface $\vec{k}_F$ must (i) be very small (or zero) at $\omega = 0$ and

\[\ldots\]
(ii) rise very rapidly to large values on some very low frequency scale, denoted by \( \Omega \), such that
\[
|\Sigma''(\vec{k}_F, \Omega)| \sim \Omega, |\Sigma''(\vec{k}_F, 0)| . \tag{58}
\]
Note that these conditions can be satisfied in our APSF model at temperatures \( T \ll \Omega_t \), where \( \Omega_t \) represents the low-energy scale \( \Omega \) and it is therefore possible to get \( \Sigma''_t'(\Omega_t + 0^+) \sim \Gamma_t \gg \Omega_t \). By contrast, these conditions can, realistically, not be satisfied in harmonic phonon exchange models, as exemplified by the harmonic Einstein model discussed above. In the latter, we have, from Eqs. (43) and (44), \( \Sigma''_h(\Omega_h + 0^+) \approx (\pi/2)\lambda_h \Omega_h \), which is comparable to the phonon energy scale for typical Eliashberg \( \lambda_h \)-values of order unity. Hence, EP-induced density of states peak effects are another important distinguishing feature between harmonic phonon and anharmonic tunneling exchange. We will now describe how this density of states peak effect arises.\(^{56}\)

Under the conditions of Eq. (58), the quasi-particle peak in \( G'' \) is rapidly damped out with increasing quasi-particle energy which, in essence, has the effect of pushing spectral weight away from the Fermi level for finite \( \omega \), of order \( \Omega \). This spectral weight removal, due to strong damping at \( \omega \sim \Omega \), occurs in addition to the spectral weight removal caused by the mass enhancement factor \( Z \). In contrast to the latter, the former spectral weight removal is not being compensated for by the reduced quasi-particle dispersion, when one averages \( G'' \) over all \( \vec{k} \) to calculate \( \rho(\omega) \). At \( |\omega| \ll \Omega \), on the other hand, spectral weight in \( G'' \) is removed only by the \( Z \)-effect which, in \( \rho(\omega) \), is being compensated for by the reduced quasi-particle dispersion. As a consequence, spectral weight will be removed from \( \rho(\omega) \) for finite \( \omega \), of order \( \Omega \), but not at very low \( \omega \), well below \( \Omega \). It is important to realize that, therefore, the resulting peak in \( \rho(\omega) \) at \( \omega = 0 \) does not arise from an enhancement of \( \rho(\omega) \) at the Fermi level, but rather from a suppression of \( \rho(\omega) \) off the Fermi level. In fact, neglecting the \( \vec{k} \)-dependence of \( \Sigma \), the density of states right at the Fermi level is essentially unchanged by the interaction, that is, from Eq. (57)
\[
\rho(0) \cong \rho(0)(0) . \tag{59}
\]
Notice also that a $\rho(\omega)$-peak, generated solely by the foregoing damping-induced spectral weight removal mechanism from a flat non-interacting density of states (i. e. from a $\rho^{(0)}(\omega) \cong \text{const at } |\omega| \sim \Omega$), will be centered right at the Fermi level $\omega = 0$. As shown in the inset in Fig. 2, this is not the case in our $T = 0$ model calculation. Here, the narrowed image of the van Hove singularity, centered at an $\omega_v HS \cong 0.02t$, is below $\Omega_t$ and superimposed on the damping-induced spectral weight suppression which occurs mainly for $|\omega| > \Omega_t$ in our model, due to the almost completely gapped $\Sigma''$ at $|\omega| < \Omega_t$, Eq. (37). However, if we change the band-filling so as to move the van Hove singularity further away from the Fermi level, then the narrowed van Hove image moves out to larger $\omega_v HS$ and gradually disappears when $\omega_v HS$ becomes comparable to $\Omega_t$ while, at the same time, the damping-induced peak at $\omega = 0$ emerges, albeit generally with less pronounced peak height.

We emphasize the foregoing especially in relation to photoemission studies of the $\vec{k}$-integrated density of states and its doping evolution in the cuprates. The foregoing considerations suggest that one needs to be very careful in the interpretation of observed $\vec{k}$-integrated density of states peaks. Such peaks need not necessarily be a manifestation of van Hove singularities, but may rather be caused by other effects, such as strongly frequency dependent damping near the Fermi level.

Also shown in Fig. 2, by the dot-dashed line, is the result of a non-self-consistent 1st order SF model calculation for $\rho(\omega)$. Here, the fully dressed internal single-electron Green’s function in Eqs. (22), (25) is replaced by the bare Green’s function at the same band filling, that is, written in the Matsubara domain, with

$$G^{(0)}(\vec{k}, i\nu) = \frac{1}{i\nu - \epsilon^{(0)}_k}.$$

Here $\epsilon^{(0)}_k$ denotes the non-interacting band, obtained from Eq. (24) with the non-interacting value of the chemical potential $\mu^{(0)}$ at the same band filling $\langle n_j \rangle^{(0)} = 0.75$. 

– 32 –
Similar 1st order calculations were first reported for this SF model in Ref. [24]. An important prediction from these early 1st order model calculations was the demonstration that the spin fluctuation exchange causes a pronounced “pseudo-gap” to open up in the density of states near the Fermi level. This pseudo-gap, i.e. a strong suppression in the density of states near $\omega = 0$, is indeed also present in our 1st order calculation, with the spectral weight depletion extending approximately from $\omega \sim 0$ up to $\omega \sim 3.8t$ in Fig. 2. However, in our self-consistent SF calculation (using a fully dressed $G$ as the internal electron line), the pseudo gap has largely disappeared, as shown by the dashed line in Fig. 2. In the $\omega$-region of the gap, where the 1st order $\rho(\omega)$ is being depleted, the self-consistent $\rho(\omega)$ is almost flat. Hence, it is not quite clear whether the original claim of pseudo-gap generation in AF spin fluctuation exchange exchange models is really tenable. At the very least, this spin fluctuation induced pseudo-gap effect, if present at finite doping, appears to be quite model dependent, that is, very sensitive to the level of approximation employed in the calculation and, possibly, to the choice of model parameters.

In Fig. 3, we show the single-hole excitation spectra$^{44}$

$$P(\vec{k}, \omega) \equiv \pi^{-1} |G''(\vec{k}, \omega)| f(\omega), \quad (61)$$

with the Fermi factor $f(\omega) \equiv 1/(e^{\beta\omega} + 1)$, for $T = 0.029t \cong \Omega_t$ and several $\vec{k}$-points along the (1, 1) direction. At all $\vec{k}$, $P(\vec{k}, \omega)$ exhibits a strong continuous "incoherent" background which is almost constant, down to $\omega \sim -2t$, and extends up to the Fermi level $\omega \equiv 0$ for $\vec{k} = \vec{k}_F$. As $\vec{k} \rightarrow \vec{k}_F(1,1)$, the expected quasi-particle peaks at energies $E_k^r < 0$ emerge from this background, sharpen, and disperse towards $E_k^r = 0$. These results are quite similar to typical angle-resolved photoemission spectroscopy (ARPES) data obtained in the cuprates at $T > T_c$.12–19,57

Notice that, at the temperature $T = 0.029t$ used here (i.e. $T \sim 110K$, assuming $t = 0.35eV$), the lattice contribution to the mass enhancement $Z_{AP}$ is already noticeably reduced by the thermal $Z$-suppression. Hence, except for the additional
line broadening caused by $\Sigma_{A'}$, the shapes and the dispersion of the quasi-particle peaks are already very similar to those in the purely electronic SF model, without coupling to lattice degrees of freedom. We emphasize that the normal-state ARPES line shapes and quasi-particle dispersion in the cuprates are measured at typical $T > T_c \sim 80 - 120 \, ^\circ K$. Even though coupling to lattice tunneling excitations may be important in shaping the quasi-particle dynamics of the cuprates at low temperatures, the tunneling excitations do not necessarily have any pronounced signature at normal state temperatures which may well be in the regime $T \sim \Omega_t$.

The quasi-particle energy band $E_{\vec{k}}$, shown in Fig. 4, also resembles typical cuprate ARPES data near $\vec{k}_F$. In particular, the very flat ("heavy mass") portions in $E_{\vec{k}}$ near $\vec{k}_F$ along the $(1,0)$-direction are very similar to recently reported quasi-particle dispersion curves along certain $\vec{k}$-directions in the cuprates. In our model, these very "heavy" sections in $E_{\vec{k}}$ are due to the close proximity of $\vec{k}_F(1,0)$ to the non-interacting band saddle point, the van Hove point $(\pi,0)$, with substantial additional band "flattening" caused by the mass enhancement $Z$. Note here that Eq. (29) has multiple solutions for $E_{\vec{k}}$ near $\vec{k}_F$, as shown in Fig. 4. The $E_{\vec{k}}$-branch crossing the Fermi level $E_{\vec{k}_F} \equiv 0$ corresponds to the quasi-particle peak in $G''(\vec{k},\omega)$. Other branches do not necessarily produce well-defined separate peaks in $G''$, because of damping.

**IV. CONCLUSION**

In summary, we have proposed a highly simplified anharmonic lattice potential model to study the effect of polaronic tunneling excitation and anti-ferromagnetic (AF) spin fluctuation exchange on the quasi-particle dynamics in a 2D single band model. The effects of both polaronic lattice tunneling and AF spin fluctuation exchange are treated in a self-consistent Migdal-type single-exchange approximation for the single-particle self-energy. At temperatures $T$ and excitation energies $\omega$ which are well below the anharmonic tunneling excitation energy scale $\Omega_t$, the
single-electron self-energy is dominated by the exchange of lattice tunneling excitations which give rise to a large and strongly isotopic mass dependent electron mass renormalization $Z$.

With increasing $T$, the lattice tunneling contribution to the electron mass enhancement, along with the isotope effect of $Z$, are rapidly suppressed and they both essentially disappear when $T$ exceeds $\Omega_t$. In the high temperature regime $T \gtrsim 2\Omega_t$, the electron mass enhancement $Z$ is completely dominated by the AF spin fluctuation exchange; the lattice tunneling excitations contribute only to the electron quasi-particle damping $|\Sigma''|$ and this damping contribution is largely $T$-independent and independent of the isotope mass. This high-temperature damping effect is therefore quite similar – and experimentally indistinguishable from – conventional disorder scattering.

Surprisingly, this anharmonic lattice contribution to the quasi-particle damping at high temperatures $T \gtrsim \Omega_t$ can be quite small compared to the electronic bandwidth, even if the anharmonic lattice tunneling fluctuations produce a very large mass enhancement at low $T$. The relatively small damping at high $T$ allows the electronic quasi-particle propagation to remain coherent at high temperatures, despite of the polaronic character of the underlying lattice dynamics. We have described in detail the “weakly bound polaron” conditions under which this behavior may occur, within the framework of a microscopic Holstein-Hubbard-type model; and we have contrasted it with the fundamentally incoherent high-$T$ behavior in “strongly bound” polaron systems.

In comparing the isotopic mass dependences of the electron mass enhancement $Z$ at low $T$ in the anharmonic tunneling exchange model versus a conventional phonon exchange model, we find that the two types of models exhibit fundamentally different behavior: The $Z$ contribution in the anharmonic tunneling exchange model is isotope dependent, whereas, in the harmonic phonon model, it is not. Furthermore, in contrast to the $T$-independent damping in the anharmonic tunneling exchange model at high $T$, the high-$T$ damping contribution in the har-
monic phonon model increases linearly with $T$. In this context the demarkation between “low $T$” and “high $T$” is given, respectively, by the tunneling energy scale $\Omega_t$ in the former and by the harmonic (Einstein or Debye) phonon energy scale in the latter model.

Based on the foregoing results, we suggest to explore the isotopic mass dependence of the low-$T$ electron mass enhancement experimentally, in order to establish whether or not anharmonic lattice tunneling excitations contribute in a significant manner to the low-energy electronic properties in the cuprate materials. Possible candidate experiments for pursuing such investigations are quasi-particle energy dispersion curves, as measured in angle-resolved photoemission spectroscopy (ARPES); Drude spectral weights, as observed in the optical conductivity; electronic specific heat; and, in the superconducting phase, the $T \to 0$ London penetration depth.

In the $\vec{k}$-integrated density of states, low-$T$ tunneling excitation exchange can produce a narrowed image of the near-Fermi-level features of the non-interacting density of states, such as, for example, a narrowed van Hove singularity peak. At finite temperatures $T \sim \Omega_t$, the van Hove peak is completely suppressed due to the thermal damping. Likewise, the quasi-particle dispersion $E_{\vec{k}}$ is largely unaffected by the anharmonic tunneling excitation exchange and the single particle spectral function, as observed in ARPES experiments, is affected only by the $T$-independent broadening, when $T \gtrsim \Omega_t$.

We note that our results concerning the low-$T$ narrowed imaging of the van Hove peak and its thermal suppression are generic to any strong-coupling low-energy boson exchange model, as demonstrated by our results for the purely electronic spin fluctuation exchange model (see Fig. 2). In boson exchange models of the type discussed here, the rapid thermal suppression of the narrowed van Hove peak in $\rho(\omega)$ is ubiquitous and entirely in line with the finding that van Hove singularities alone are not sufficient to bring about or substantially enhance
high-$T_c$ pairing instabilities. Our results thus strongly support the notion\textsuperscript{58} that a conjectured "van Hove scenario"\textsuperscript{59} of high-$T_c$ superconductivity does not exist.

To the extent that the cuprates can be described in terms of this type of low-energy “tunneling boson” exchange picture, we emphasize that the observed normal-state mass enhancements\textsuperscript{12−19} $Z(T) \sim 2 - 4$ may substantially underestimate the true bosonic coupling strength\textsuperscript{44}, $\lambda \equiv Z(T = 0) - 1$. As shown here, $Z(T) \ll Z(T = 0)$ if the normal state measurement temperature $T$ (e. g. $T > T_c \gtrsim 80 - 120 K$ in the cuprates!) exceeds the relevant boson energy scale $\Omega$. Also, for $T \ll \Omega$, the full $Z(T=0)$ will be observable only within a very narrow energy range ($\ll \Omega$) around the Fermi level, which could well be below current limits of resolution.\textsuperscript{12−19} In high-$T_c$ systems where $\Omega_t \gtrsim T_c$ for $T \ll T_c$, it needs to be explored to what extent the full normal-state value of $Z(T=0)$ is observable in the presence of a superconducting gap $\Delta$ with $\Delta \gtrsim \Omega$. Finally, we note that a strongly $T$-dependent $Z$ has important implications for the $T$-dependence of quasi-particle lifetimes $\tau$, since $1/\tau \equiv |\Sigma''|/Z$ is renormalized by $Z$.

Given sufficient energy resolution, the full $T=0$ normal-state mass enhancement should be observable in systems where $T_c \ll \Omega$, at temperatures $T$ well below $\Omega$. From the $T$-dependence of $Z(T)$, the relevant boson energy scale can then be established. Also, the possible observation of the $\rho(\omega)$-resonance peak should be explored. The resonance is observable by either direct or inverse angle-integrated photoemission spectroscopy, depending on the resonance peak position $\omega_{vHs}$ relative to the Fermi level $\omega = 0$. The resonance can also cause a low-energy gap structure, on an energy scale of order $|\omega_{vHs}|$, in the two-particle electronic response functions.

To put our model results in a more general perspective, we note that the specific shape of the spectral weight depletion around the Fermi level $\omega = 0$ in the self-energy [see Eq. (37)] is obviously model dependent. However, the qualitative feature of its existence is characteristic of the low-energy behavior of any Fermi liquid. What is unusual about this Fermi liquid behavior in the lattice tunneling
self-energy studied here, is the fact that the Fermi liquid character begins to break
down already at a very a low excitation energy ($\omega$) and temperature scale, set
by the tunneling energy $\Omega_t$. This can, but need not be lower than all other
electronic or lattice energy scales, because of the great sensitivity of tunneling
matrix elements to small changes in the tunneling barriers. Thus, the tunneling
energy scale (i) could vary substantially between different materials; (ii) within
the same parent material, it could vary substantially as a function of doping level;
and (iii) it could well be lower than either the harmonic phonon or even the
superconducting $T_c$ scale in the cuprates.

These last features of our model are generic to the low-energy physics of
strongly correlated polaronic electron systems; they do not depend on the model
simplifications we have introduced here. What is quite likely to change in a more
realistic polaron model is the structure of the anharmonic lattice dynamics, as re-
lected e. g. in the $\omega$- and $\vec{q}$-dependence of $V_{AP}$. This, in turn, will have important
ramifications for the details of the $T$- and $\omega$-dependence of the self-energy in such
systems.

Lastly, we should also emphasize that the Hubbard-type local Coulomb cor-
relations play a central role in such a polaronic picture, for two reasons. Firstly,
the local Coulomb repulsion is important to prevent the formation of bi-polarons
and hence, to preserve the essentially fermionic character of the quasi-particles.
Secondly, the Coulomb correlations are the origin of the AF spin correlations in
the nearly $\frac{1}{2}$-filled regime. As discussed previously, the AF spin correlations
are essential to allow doping induced carriers to form polarons at much weaker
EP coupling strengths than would be required in weakly correlated systems. As a
consequence, the resulting polaronic system can have much lower tunneling barri-
ers and hence, reach much larger $\Omega_t$-scales than one would estimate for weakly /
un-correlated small-polaron systems.

Note that the latter is crucial if one wants to apply such a polaronic picture
to the cuprates. On the one hand, one will need low tunneling energy scales in
order to explain the breakdown of Fermi liquid behavior down to very low temper-
atures, down to, say, \( \sim 10K \), in some cuprate systems; on the other hand, one will
need large tunneling energy scales to to explain the unusual \( T \)-dependences of the
quasi-particle and transport dynamics which are found over very large tempera-
ture scales, up to \( \sim 100 - 1000K \). A lattice excitation spectrum covering several
orders of magnitude of excitation energy will therefore be essential. This, again,
emphasizes the importance of more realistic models of the polaronic lattice dy-
namics and will require further study.

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FIGURE CAPTIONS

FIG. 1. Mass enhancement \( Z = 1 - \partial_\omega \Sigma'(\vec{k}_F, \omega = 0) \) vs. temperature \( T \) at the Fermi surface point \( \vec{k}_F(1, 1) \approx 0.44(\pi, \pi) \) in the APSF model, with \( V \equiv V_{AP} + V_{SF} \) in Eq. (25), (upper full line) and in the purely electronic SF model, with \( V \equiv V_{SF} \) in Eq. (25) (lower full line). Also shown is \( Z_{AP} = -\partial_\omega \Sigma'_{AP}(\omega = 0) \) vs. \( T \) in the APSF model (dashed line), where \( \Sigma'_{AP} \) is the \( V_{AP} \)-contribution to \( \Sigma' \) in the APSF model. The model parameters are given in the text in Sec. III.A, following Eq. (46).

FIG. 2. Density of states \( \rho(\omega) \) vs. energy \( \omega \) at temperature \( T \approx \Omega_t \). APSF (full line) and SF (dashed line) are the results, for the respective models, as defined in Fig. 1. The results labeled SF1 (dot-dash line) are results of non-self-consistent 1st order calculations for the SF model, as described in text. Inset: APSF and SF results for \( \rho(\omega) \) vs. \( \omega \) near \( \omega = 0 \) at \( T \approx \Omega_t \) and \( T = 0 \). The other model parameters are the same as used in FIG. 1.

FIG. 3. Hole excitation spectra \( P(\vec{k}, \omega) \) vs. energy \( \omega \) in the APSF model [with \( V \equiv V_{AP} + V_{SF} \) in Eq. (25)] for \( \vec{k} = (k_x, k_x) \) at \( k_x \)-values indicated, at temperature \( T \approx \Omega_t \). Spectra are off-set by successive vertical shifts, with dashed lines showing zero intensity. The other model parameters are the same as used in FIG. 1.

FIG. 4. Quasi-particle bands \( E_{\vec{k}} \) vs. wavevector \( \vec{k} \) in the APSF model [with \( V \equiv V_{AP} + V_{SF} \) in Eq. (25), full line] and in the non-interacting system [\( V \equiv 0 \), dashed line], along several directions in the 2D Brillouin zone, both at the same electron concentration \( \langle n_j \rangle = 0.75 \), at temperature \( T \approx \Omega_t \). The other model parameters are the same as used in FIG. 1.
\[ \rho(\omega) / t^{-1} \]

\[ \text{APSF} \]

\[ \frac{1}{\omega t} \]

\[ T=0 \]

\[ T=0.029t \]
\( E_{\kappa/t} \)

\[
\begin{array}{cccc}
-4 & 0 & 4 & 8 \\
(0,0) & (\pi,0) & (0,\pi) & (\pi,\pi) \\
\end{array}
\]