Electronic properties of the pseudogap system 
\((TaSe_4)_2I\)

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Abstract.
The room temperature “metallic” properties of the quasi-one-dimensional material \((TaSe_4)_2I\) differ markedly from those expected of either a Fermi or a Luttinger Liquid, showing strong signs of a suppression of the density of states at the Fermi level. We present evidence for the existence of strong quasi–static fluctuations of structural order with long correlation length. These fluctuations produce a pseudogap in the density of states. We compute the temperature dependence of the optical and DC conductivities of \((TaSe_4)_2I\) in its conducting phase, the nature of its core hole spectra, the NMR Knight Shift and relaxation rate. Predictions for these quantities are made on the basis of a Lee, Rice and Anderson model. This model represents the simplest theory of a pseudogap, and gives satisfactory agreement with experiment in the cases where comparisons can be made. In contrast, the predictions of a strongly correlated (Luttinger Liquid) model appear to to contradict the data. The chief remaining discrepancy is that the gap deduced from transport quantities is less than that observed in photoemission. We discuss some possibilities for resolving this issue.

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Short title: Pseudogap in \((TaSe_4)_2I\).

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1. Introduction

(TaSe$_4$)$_2$I is among the most widely studied of quasi one-dimensional materials. First synthesized in 1984 [1], it provides a good example of a “metallic” system undergoing a Peierls transition to a nearly commensurate charge density wave ground state. It is unusual among low dimensional systems in the uncommonly high temperature (263 K) at which it becomes ordered, and in the way in which that ordering affects its room temperature properties. It has attracted interest as a Luttinger liquid candidate, based on its photoemission spectrum [2], [3]. We argued in an earlier paper [4] that none of the observations on (TaSe$_4$)$_2$I are really consistent with the Luttinger picture, and that the photoemission is best explained by its proximity to a charge density wave state — the energy scale associated with the gap which opens in the charge density wave state is clearly visible in the room temperature properties of (TaSe$_4$)$_2$I, as was shown by early measurements of magnetic susceptibility [5]. (TaSe$_4$)$_2$I is clearly a ‘pseudogap’ system.

Below 263 K, the resistivity of (TaSe$_4$)$_2$I shows an activated behavior, and measurements of its optical conductivity and of the dispersing features measured in angle-resolved photoemission (ARPES) spectra also give evidence of a gap. Strangely however, the gap (or, above 263 K the pseudogap) measured by different experiments is not of the same size, as is illustrated in Table 1, where gaps and their corresponding mean-field transition transition temperatures are listed.

|                     | $\Delta$  | $T_{3D}$ | $T_{MF}$ |
|---------------------|-----------|----------|----------|
| DC Conductivity     | 180 meV/2100 K | 263 K    | —        |
| Optical Conductivity| 200 meV/2300 K | —       | —        |
| ARPES               | 520 meV/6000 K | —       | 892 K    |
| Magnetic Susceptibility | —         | —       | 860 K    |

Roughly speaking, the gap in ARPES spectra is 2 to 3 times that in other experiments. We discuss below how this discrepancy may be resolved.

Coincidentally, observation of the pseudogap state in underdoped high-$T_c$ superconductors has caused great excitement. The nature of this state is presently intensely debated, with no consensus having been reached. In this context, it is important to look in some detail at (TaSe$_4$)$_2$I which, we believe, is a much simpler pseudogap material. In fact we will contend that its properties, with the single exception of the gap discrepancy, can be understood in a straightforward, and even rather crude, theory.

The dispersing features measured by ARPES in the conducting phase were found to be quite well described by a simple Lee, Rice and Anderson (LRA) model in which
the fluctuations of lattice order associated with the Peierls transition are viewed as a
temperature dependant ensemble of static potentials in which the electrons move [6],
and electron–electron interaction is explicitly not included.

In this paper we extend the analysis begun in [4] to optical and DC conductivities,
making predictions for the temperature dependence of these quantities in the conducting
phase on the basis of the same simple LRA model. We will also discuss what might be
learned from NMR and core hole photoemission experiments on (TaSe$_4$)$_2$I, considering in
particular what might be established about spin–charge separation from the comparison
of the two. In all cases we compare these predictions both with existing experimental
data and with the behavior expected of models based on strong electron–electron
interaction. For greater readability, ancillary technical details are given in appendices.

2. The Lee, Rice and Anderson model

Conduction in (TaSe$_4$)$_2$I takes place along one-dimensional chains of Ta atoms [7]. The
material undergoes a Peierls transition at $T_c = 263K$ to a state where the lattice is
distorted by a condensed transverse acoustic phonon mode. This may be thought of
in simple terms as a slightly incommensurate tetramerization of the tantalum atoms
perpendicular to the chain axis. Superlattice reflections appear in X–Ray spectra at
$\vec{q} = (\pm 0.05, \pm 0.05, \pm 1.085)$, confirming incommensurate charge density wave order not
quite aligned with the chain axis [8]. In the chain, this corresponds very nearly to a $2k_F$
fluctuation.

The proper model for what is then a one-dimensional electron–phonon problem is
given by the Fröhlich Hamiltonian

$$H = \sum_k \epsilon(k)c_k^\dagger c_k + \sum_q \omega(q)b_q^\dagger b_q + \frac{1}{\sqrt{L}} \sum_{q,k} g(q)c_{k+q}^\dagger c_k u_q,$$

where

$$u(q) = \frac{1}{\sqrt{2\omega(q)}}(b_q^\dagger + b_{-q}),$$

and $c_k^\dagger$ and $b_q^\dagger$ are (respectively) creation operators for electrons and phonons with
dispersion $\epsilon(k)$ and $\omega(q)$. $u_q$ is the Fourier transform of the lattice displacement, and
$g(q)$ the electron-ion coupling. Since electron spin enters into the problem only in
appropriate factors of two, it will be suppressed in our notation.

The physics of this Hamiltonian has been widely studied for many years and is
highly nontrivial. It is well known both that the one dimensional lattice is unstable
against distortion, and that thermodynamic fluctuations prevent a transition to a state
with long range order from occurring at finite temperature in any truly one–dimensional
system.
The possibility of phonons with wave number \( Q = 2k_F \) decaying into zero energy particle–hole pairs leads to softening of the phonon spectrum for \( Q \approx 2k_F \), and at a mean field level the system described by the one–dimensional Fröhlich Hamiltonian Eq. (1) undergoes a transition to a fully ordered charge density wave state at the temperature \( T_{MF} \) for which the frequency of the \( Q = 2k_F \) phonon mode goes to zero \([4]\). This temperature is determined by the strength of electron–phonon coupling \( g(2k_F) \), and is of the same order as the gap developed in the charge density wave state at absolute zero. Within the set of approximations usual for BCS theory one has \( 2\Delta = 3.5k_B T_{MF} \) but for real materials this relation is seldom exact. The three-dimensional charge density wave transition which occurs in \((\text{TaSe}_4)_2\text{I}\) and other similar compounds is stabilized by interaction between different metallic chains, but occurs at a temperature much smaller than the gap energy, as can be seen in Table 1 where \( T_{MF} \) is certainly well above the experimental transition temperature.

In the spirit of LRA, we identified the transition temperature \( T_c = T_{3D} = 263K \) with a crossover from a three dimensional Peierls–distorted mean field charge density wave state described by

\[
H_{MF} = \sum_k \epsilon(k) c_k^\dagger c_k + \sum_k [\Delta^* c_{-k+2k_F}^\dagger c_k + \Delta c_{-k+2k_F}^\dagger c_{-k}] \\
\Delta = \frac{1}{\sqrt{L}} g(2k_F) \langle u_{2k_F} \rangle.
\]

(2)

(3)

to a state in which there are essentially uncorrelated fluctuations of charge density wave order on individual chains. We make no attempt to accurately describe the way in which this dimensional crossover takes place. Fluctuation effects above \( T_{3D} \) are taken into account in the simplest possible way consistent with a mean–field ground state, replacing the order parameter for the Peierls distortion of the lattice \( \Delta = \frac{1}{\sqrt{L}} g(2k_F) \langle u_{2k_F} \rangle \) by a static external field which has a non–vanishing expectation value for other momenta not exactly equal to \( 2k_F \):

\[
H_{LRA} = \sum_k \epsilon(k) c_k^\dagger c_k + \sum_{Q,k'} [\Psi_Q^* c_{Q+k'}^\dagger c_{Q-k} + \Psi_Q c_{-Q-k'} c_{-Q+k}] \\
\Psi_Q = \frac{1}{\sqrt{L}} g(Q) \langle u(Q) \rangle.
\]

(4)

(5)

The classical field \( \Psi_Q \) belongs to a thermal ensemble of potentials characterized by a mean square “gap” scale \( \langle \psi^2(T) \rangle \) reflecting the size of fluctuations of lattice disorder, and an inverse coherence length \( \xi^{-1}(T) \).

Since the main purpose of this paper is to explore the LRA model as a phenomenology for \((\text{TaSe}_4)_2\text{I}\) we consign the derivation of the single-particle Green’s function for electrons moving in this static phonon field to [Appendix A] and reproduce
here only the result

\[ G(k, \omega_n)^{-1} = i\omega_n - \epsilon(k) - \frac{\langle \psi^2(T) \rangle}{i\omega_n + \epsilon(k) \pm iv_f \xi^{-1}(T)}. \]

where the choice of sign \( \pm iv_f \xi^{-1}(T) \) is made according to whether we continue to the upper or lower half plane. For convenience we have set \( \hbar = 1 \).

Determining the temperature dependence of \( \langle \psi^2(T) \rangle \) and \( \xi^{-1}(T) \) forms an essentially independent problem; for a fully self-consistent phenomenology they should be found from experiment. The scale of \( \langle \psi^2(T) \rangle \) is set by the size of the mean gap at \( T = 0 \), and it varies little over the range of temperatures in which we can apply the LRA theory to experiments on \((\text{TaSe}_4)_2\text{I}\), i.e. \( 263 < T < 430K \). In contrast \( \xi^{-1}(T) \) varies quite strongly with temperature, and becomes extremely small at the transition temperature \( T_{3D} \). For all experimentally accessible temperatures \( v_f \xi^{-1}(T) \ll \sqrt{\langle \psi^2(T) \rangle} \). Our parameterization of the model is discussed in more detail in Appendix B.

In what follows we will use a spectral representation of the electrons

\[ A(k, \omega) = \frac{2v_F \xi^{-1}(T) \langle \psi^2(T) \rangle}{[\omega^2 - \epsilon(k)^2 - \langle \psi^2(T) \rangle]^2 + v_F^2 \xi^{-2}(T)[\omega - \epsilon(k)]^2}. \]

All the anomalous features of the room temperature ARPES data are present in this spectral function. In particular it predicts the broad dispersing features, and “quasigap” structure observed by Terassi et al.\[3\].

It is important to note that the results of this paper assume the validity of (7) and nothing further, since all experimental quantities can be expressed as integrals over the spectral functions. Since this equation can be directly compared with experiment, we may regard our theory in two different ways. On the one hand, it may be viewed as a phenomenology in which the spectral function is taken from one experiment (ARPES) and used to develop a picture of several experiments, or it may be viewed as a direct test of the LRA model against experiment, without prejudice as to the suitability of LRA as a solution to the Fröhlich Hamiltonian.

3. Previous Work

For completeness, we review previous work on the application of these equations to explain experimental data. An example of a fit to a room temperature ARPES spectrum for \((\text{TaSe}_4)_2\text{I}\) made on this basis in Ref.\[4\] is shown in Figure\[2\]. A fit to the temperature dependence of the uniform magnetic susceptibility of \((\text{TaSe}_4)_2\text{I}\) by Johnston et al.\[5\], is given in Figure\[3\]. In both cases, the agreement of theory and experiment is excellent.
4. DC Resistivity

The DC resistivity $\rho(T)$ of (TaSe$_4$)$_2$I is usually presented in an Arrhenius plot so as to extract an ordering temperature $T_{3D}$ and an activation energy $\Delta_0$ for the charge density wave state. For temperatures above $T_{3D}$ the data plotted in this form show no upturn — in fact the resistivity becomes nearly temperature independent, decreasing slowly over all higher measured temperatures [10]. This contradicts our expectations of an ordinary metal, where most scattering mechanisms increase in effectiveness with increasing temperature, and an upturn in $\rho(T)$ is expected on the closing of the gap.

In the LRA liquid we anticipate that scattering of electrons from fluctuations of charge density order will have two effects on conductivity: the suppression of the density of states at the Fermi energy, and the imposition of a finite lifetime on electrons propagating in momentum eigenstates along the chains. The former is reflected in the pseudogap visible in photoemission spectra and the spectral function Equation (7), the latter in the large temperature-dependent width of the dispersing features in the spectral functions. The temperature dependence of the conductivity of will therefore depend on the interplay between the gap and lifetime effects as parametrized by $\langle \psi^2(T) \rangle$ and $\xi^{-1}(T)$.

We calculate the intrinsic DC conductivity of an LRA liquid directly from a current–current correlation function. The results of the usual Kubo formalism, evaluated to first order, may be expressed directly in terms of the spectral function of the system under consideration as [11]:

$$
\sigma^{(1)}_0 = -\frac{e^2}{2m^2} \int_{-\infty}^{\infty} \frac{d\omega}{2\pi} \frac{\partial n_f(\omega)}{\partial \omega} \sum_k k^2 |A(k, \omega)|^2
$$

We evaluate the sum over $k$ as a contour integral and perform the final integral over $\omega$ numerically. We do not include disorder in our calculations in this paper, and the DC conductivity is of course sensitive to disorder. We therefore add a small temperature independent part to the inverse coherence length $\xi^{-1}(T)$, which we chose to be $\xi^{-1}(300K)$. This affects the temperature dependence of the conductivity only near $T_{3D}$. In order to present consistent results we will include this correction in later calculations of optical conductivities.

Theory and experiment are shown in the interesting range from 264K to 430K in Fig. 4. There is qualitative agreement, in that the unusual slow decrease with temperature is reproduced. However, it is clear that a proper treatment of the crossover to three dimensions is needed to fit the data near $T_{3D}$.

To understand the qualitatively behavior of $\rho(T)$, we can make an estimate of the scale of the temperature dependence somewhat in the spirit of the Drude model:

$$
\sigma(T) \sim D_{LRA}(\epsilon_f) \times \tau_{LRA},
$$
where $\tau_{LRA}$ is the effective lifetime of the electrons and $D_{LRA}(\epsilon_f)$, the density of states at the Fermi energy, has been chosen as a representative measure of the degree to which the gap has filled.

An expression for $D_{LRA}(\omega)$ can be found analytically from (7); for $\omega = \epsilon_f$ it has the simple form

$$D_{LRA}(\epsilon_f) = \frac{v_f \xi^{-1}(T)}{\langle \psi^2(T) \rangle} \approx \frac{v_f \xi^{-1}(T)}{\langle \psi^2(T) \rangle}$$

(10)

Naively, we might expect $1/\tau_{LRA}$ to be given by the imaginary part of the self energy of an electron at $k = k_f$, $\omega = 0$, but this diverges for $\xi \to 0$, while the reciprocal of the real electron lifetime should tend to zero. However in the limit where $v_f \xi^{-1}(T)/\sqrt{\langle \psi^2(T) \rangle} \to 0$ it is possible to show that the spectral function of Eq. (7)) can be rewritten as the sum of two Lorentzians, with $v_f \xi^{-1}(T)/2$ playing the role of a lifetime (peak width). A naive prediction for the DC conductivity would then be:

$$\sigma(T) \sim \frac{1}{\langle \psi^2(T) \rangle}.$$  

(11)

Since $\langle \psi^2(T) \rangle$ decreases only slightly over experimentally relevant temperatures, this represents a weakly temperature-dependent increasing conductivity, as is observed. But note that the conductivity we calculate is anything but temperature-independent over the remainder of the (greater) range of temperatures which we may access in our model. By fitting the numerical results we find it is rather well described by a high power law in the reduced temperature $(T/T_{MF})^x$, $x \approx 10$, with the weak temperature dependence of the conductivity at low temperatures being due to its suppression by many factors of $T/T_{MF}$.

Thus the very weakly temperature dependent DC conductivity is well explained by a cancellation of density-of-states and lifetime effects. This fails to capture the interesting step-like feature seen at the transition temperature in an Arrhenius plot. This is not surprising, as the dimensional crossover is not included in a realistic fashion in our theory. This (near) independence of DC conductivity on temperature over so large a range of temperatures is sufficiently unusual that we consider it to be a striking confirmation of the LRA theory.

5. Optical conductivity of the LRA Liquid

The optical conductivity of $(\text{TaSe}_4)_2\text{I}$ has been measured over a range of temperatures \cite{8} and also shows a surprising lack of evolution with temperature.

A truly gapped state, such as that described by Eq. (2) cannot support charge carrying excitations (or indeed any excitations) at energies less than the $2\Delta$ needed to promote charge across the gap. The measured optical conductivity should therefore
“turn on” abruptly at $\omega \approx 2\Delta$. Since the density of states diverges immediately above and below the gap, we expect a very pronounced asymmetric peak at $\omega = 2\Delta$ with almost all weight on the high energy side.

Such a peak is indeed observed in the charge density wave state of (TaSe$_4$)$_2$I. However, it is rather less asymmetric than might have been expected. Away from the maximum the spectra grow as $\omega^2$ on the low– and fall away as $1/\omega^3$ on the high–energy side. Since we are only interested in the excitations from the band of electrons which carry currents in (TaSe$_4$)$_2$I, we will ignore the presumably interband contribution which sets in beyond $1.2eV$.

In a mean-field-like picture, we would expect the feature at $\omega \approx 2\Delta \approx 400meV$ to become weaker, broader, and migrate to lower energies as the temperature is raised and the gap closes. The first two of these expectations are fulfilled, but over the range of temperatures $15K - 400K$ the position of the maximum changes by a few $meV$ only, and not by the $\approx 120meV$ that might have been expected from our parameterization of the model.

The only qualitative change in the peak as (TaSe$_4$)$_2$I is heated through $T_{3D}$ is the loss of the simple $\omega^2$ behavior on the low energy side — on a log–log scale the peak grows a small shoulder at a little below $\Delta$. On the high energy side the peak still falls away as $1/\omega^3$.

In fact the Hamiltonian in Eq. 2 is not adequate by itself to describe the dynamics of the ordered state. The lattice distortion may vary slowly in space and time [13], leading to low energy collective modes in the charge density wave which are observed at finite frequency in Blue Bronze even in its conducting phase [14]. Since we are mostly concerned with pseudogap effects in the single–electron properties of (TaSe$_4$)$_2$I however, we will not consider such collective excitations here.

Under this approximation, the optical conductivity of the Lee, Rice and Anderson model can be calculated directly from a Kubo formula expressed in terms of electron Green’s functions, in the same way as the DC conductivity. In this case we start from

$$\sigma(\omega) = -\frac{e^2}{2m^2} \int_{-\infty}^{\infty} \frac{d\epsilon}{2\pi} \left[ \frac{n_f(\epsilon + \omega) - n_f(\epsilon)}{\omega} \right] \sum_k k^2 A(k, \epsilon) A(k, \epsilon + \omega)$$

which obviously has Eq. (8) has its $\omega \rightarrow 0$ limit. Once again we perform the sum over $k$ analytically and the integration over $\omega$ numerically. Typical results are presented on a log–log scale in Figure 5. They may be characterized by

- Lorentzian peak at $\omega = 0$ with width of the order the naive quasiparticle inverse–lifetime $v_F\xi^{-1}(T)$.
- Strongly suppressed response over the range of energies $\omega \approx v_F\xi^{-1}(T) \rightarrow \sqrt{\langle \psi^2(T) \rangle - v_F^2\xi^{-1}(T)^2}$.
- Shoulder at $\omega \approx \sqrt{\langle \psi^2(T) \rangle - v_F^2\xi^{-1}(T)^2}$ (for temperatures sufficiently close to $T_{3D}$).
• Sharp asymmetric peak at $\omega \approx \sqrt{\langle \psi^2(T) \rangle} - v_F^2\xi^{-1}(T)^2$ with temperature dependent position, width and height.

• Asymptotic decay as $1/\omega^3$ at high frequencies.

These features of the spectra and their temperature dependences are again in good qualitative agreement with those taken on $(TaSe_4)_2I$, although it is important to note that we have been forced to abandon the value of the zero temperature gap $\Delta_0 = 0.52eV$ required to fit photoemission in favour of the smaller value $\Delta_0 = 0.2eV$ suggested by transport measurements. This value is listed in Table 1. We have explicitly checked that the $\omega \to 0$ limit of the predicted optical conductivity matches our prediction for the DC conductivity, providing a useful self-consistency check on each calculation.

The important differences been model and experimental spectra are

• Greater temperature dependence of the peak position.

• Lack of weight within the gap — experimental spectra have more weight within the “gap” especially at low temperatures.

Interestingly recent higher resolution photoemission spectra for $(TaSe_4)_2I$ also show less temperature dependence in the peak position than the earlier data which we fitted in terms of the LRA model [15]. Without attempting a detailed analysis, we note that optical conductivity spectra taken on Blue Bronze are qualitatively very similar to those taken on $(TaSe_4)_2I$. Spectra for the family of organic quasi one-dimensional systems $(TMTSF)_2X$, on the other hand, show important differences in detail [16].

We wish to stress that measurement of the different gap scales by different experiments, and the excess of weight in the gap are problems not of the conducting phase only, but also need to be addressed in the ordered phase. To do this it may be necessary a) to go beyond the approximation of static lattice distortion which underlies both the mean field theory of the ordered state and the LRA model and b) to include the effects of electron–electron interaction and/or impurities in a more careful way.

One way of obtaining a better fit to optical conductivity spectra in the ordered phase would be to convolute the expected mean field response function (which is singular at $2\Delta$) with a Lorentzian “damping function” [17]. This however leads to the transfer of rather too much weight into the subgap region ($\omega < 2\Delta$). It has been argued that the effect of both thermal and quantum fluctuations in the ordered phase can be modeled with a zero mean “white noise” potential (i.e. one with only delta function correlations in real space) [18]. Predictions based on this model have been successfully applied to optical conductivity spectra for the charge density wave states in KCP $(K_2Pt(CN)_4Br_{0.3}H_2O)$ [19] and Blue Bronze $(KMnO_3)$ [20]. In the case of $(TaSe_4)_2I$ [21], while the spectra showed some deviations from the predicted behavior, the temperature dependence of spectra for $T < T_{3D}, \omega < 2\Delta$ led the authors to conclude that lattice fluctuations are indeed an important effect, even in the fully ordered charge density wave state.
6. Comparison with Strongly Correlated Models

The properties of (quasi) one-dimensional strongly correlated electron systems have been studied theoretically for more than twenty years and good reviews exist [21]. We shall only highlight the transport properties of interacting systems which differ radically from non-interacting ones in ways which are relevant for the experiments discussed above.

We may characterize the Luttinger Liquid (LL) state as a) spin–charge separated — low energy spin and charge excitations are independent of one another; b) gapless — low spin and charge excitations are bosonic collective modes with “acoustic” dispersion \( \omega_{\rho(\sigma)} = v_{\rho(\sigma)} |q| \); and c) critical — all correlation functions decay with power laws determined by two parameters interaction \( K_\rho \) and \( K_\sigma \). (We assume spin rotation symmetry below, in which case \( K_\sigma \equiv 1 \). For a recent review of LL physics, see [22]).

These properties are most conveniently illustrated by the asymptotic form of the single particle correlation function

\[
G(x,t) = \frac{1}{2\pi} \left[ \frac{e^{ik_fx}}{\sqrt{x-v_\rho t}\sqrt{x-v_\sigma t}} + \frac{e^{-ik_fx}}{\sqrt{x+v_\rho t}\sqrt{x+v_\sigma t}} \right] \left[ \frac{\Lambda^2}{x^2-v_\rho^2 t^2} \right]^\theta
\]

(13)

where \( x, v_\rho t, v_\sigma t \gg \Lambda \), a cutoff (interaction range), and

\[
\theta = \frac{1}{8} \sqrt{K_\rho + \frac{1}{K_\rho} - 2}
\]

(14)

Local repulsive interactions lead to \( 1/2 < K_\rho < 1 \) \([0 < \theta < 1/8\sqrt{2}]\).

It is immediately evident from this correlation function that the Luttinger Liquid does not support Fermionic quasiparticles — it has no pole structure in the propagator and therefore no Fermi surface. That the density of states vanishes as a power law

\[
D(\omega) \sim \omega^{2\theta},
\]

and that the Fermi surface “step” is replaced by a weaker algebraic decay \(|n(k) - 1/2| \sim |k - k_f|^{2\theta}\) follows from setting \( x = 0 \) \((t = 0)\) in (13) and Fourier transforming on \( t(x) \). In fact the spectral properties of the models leading to (13) have been worked out in some detail [23], and represent a convolution of the responses of the spin and charge sectors. For a general “universal” parametrization of the interaction, the single electron spectral function has two singularities, dispersing as \( v_\rho (k - k_f) \) and \( v_\sigma (k - k_f) \). The extent to which the spin–charge separated model is not universal in its spectral properties is discussed in [24].

Like the free electron gas, the Luttinger liquid is a perfect conductor, and the finite conductivity of any experimental realization of a Luttinger liquid would be determined by the effect of additional terms in the Hamiltonian arising from disorder or coupling to external fields (crystal field, phonons, etc.). These are strongly renormalized by
interaction \[23\], and scaling arguments lead to power law temperature dependence of 
\( \sigma_0 \), and power law behavior in \( \omega \) for \( \sigma(\omega) \) arising from those (Umklapp) terms which 
open a gap to charge excitations \[21, 26\].

\[
\rho(T) \sim T^{2-\nu} \tag{16}
\]
\[
\sigma(\omega) \sim \omega^{-\nu} \tag{17}
\]
\[
\nu = 4n^2K_\rho - 5 \tag{18}
\]

where \( n \) is the commensurability of the system (inverse of number of electrons per site).
\((\text{TaSe}_4)_2\text{I}\) is naively a quarter filled system, in which case \( n = 2 \) and

\[
\nu = 16K_\rho - 5 \tag{19}
\]

Room temperature optical conductivity and ARPES measurements show clear evidence
of a gap scale \( \Delta \), which means that the conducting phase of \((\text{TaSe}_4)_2\text{I}\) cannot be a LL
by our definitions above. Nonetheless we might can still look for evidence of strong
correlation effects for \( \omega \gg 2\Delta \), with the understanding that structure at lower energies
will be non-universal and rather more complicated.

Fitting the \( \omega^{-3} \) tail of the optical conductivity leads to the value \( K_\rho = 1/2 \) – the
extreme limit of what may be accomplished with local electron–electron interaction, but
not incompatible with strong electron–phonon interaction. In this case we expect a gap
to open in the spin sector and a renormalization

\[
\tilde{K}_\rho = \sqrt{\frac{m}{m^*}}K_\rho \tag{20}
\]

where we have followed the convention usual in CDW literature of associating
a renormalized electron mass \( m^* \) with the dynamics of the charge density wave. Empirically this may be as much as a few hundred times \( m \).

Self consistently using the value \( K_\rho = 1/2 \) in (16) we would then anticipate
\( \sigma_0 \sim 1/T \), which is entirely incompatible with the monotonically increasing conductivity measured experimentally. To attempt to extract a value of \( K_\rho \) by fitting the vanishing of the density of states at the chemical potential with the form 15 is clearly perverse in a system with so large a gap, and leads to even more extreme values of \( K_\rho \approx 1/3 \).

It is worthwhile noting that the conductivity calculated above is the the hydrodynamic conductivity of the liquid (the response of an isolated system in equilibrium to an applied field), and not an experimental conductance. Predictions for the Landauer (two terminal) conductance of an isolated LL depend on how one considers it to be coupled to the current carrying leads of the experimental apparatus \[27, 28\]. As far as we are aware, the question of how a real system of many chains couples to external current carrying leads has not been considered in detail by any author.

The LL is thus clearly a poor candidate for describing the low energy properties of
the conducting phase of \((\text{TaSe}_4)_2\text{I}\): experiment shows clear evidence of a pseudogap at
room temperature in both spin and charge channels, and even above this gap energy scale it does not obey the universal properties scaling expected of a such a model.

Another paradigm for a one–dimensional conducting state is the Luther–Emery (LE) Liquid, which is spin–charge separated and has the same charge excitations as a LL, but a gap to spin excitations. Moreover, while a LL supports both charge density wave and spin density wave excitations decaying with the same power law, the spin gap in the LE Liquid singles out charge density wave fluctuations, making it a natural candidate for describing quasi one-dimensional charge density wave systems.

The LE Liquid should respond in the same way as the LL in all responses which couple to charge alone, and so it will have the same ideal hydrodynamic conductivity as a LL or a free electron gas. An important consequence of this is that its optical conductivity should obey the same power law behavior as that of a LL. The spin–gap is felt however, whenever a probe measures spin excitations (susceptibility measurements) and also if it couples directly to electrons, as in photoemission, tunneling experiments, and two terminal conductances, so all of these should show evidence of a (quasi–)gap. As both charge and spin sensitive probes reveal clear evidence of a gap in (TaSe₄)₂I, we do not feel that there are any strong arguments in favour of the LE Liquid in this case. That the LE Liquid may provide a rather better description of Blue Bronze has been suggested by Voit [12].

7. Core Hole Spectra

Core level X-Ray photoemission spectroscopy (XPS) provides a useful probe of the structure of a material, and of the low energy excitations of any charge carriers present in it. Generically these spectra have the form of a set of lines in an incoherent background, at energies many electron volts below the chemical potential. Because the wavefunctions of the electronic core levels are physically very small, they provide an essentially local probe of the structure of the material, with shifts in individual lines providing information about changes in the electric field and charge susceptibility at the sites of individual atoms.

The details of the lineshape of electrons emitted from core levels also depend sensitively on the low energy excitations of any free charge. These excitations are in turn dominated by many–body effects and the asymmetries observed in lineshapes for metals are closely related to another much studied problem – the “Fermi Edge Singularity” (FES) in X–ray absorption. We will argue that, taken in conjunction with a complementary local probe of low energy spin excitations such as NMR, XPS (or, with some modification to our arguments, the FES) offers a novel means of distinguishing between different metallic and conducting phases.

The calculation of many body effects in core level and X–ray edge response in three
dimensions for a Fermi Liquid has been extensively studied in a body of work commonly referred to as MND (Mahan–Nozières–Dominicis) theory [29].

In the case of ordinary metals it is enough to consider the noninteracting problem.

\[ H = H_0 + V \]

\[ H_0 = \sum_k \epsilon(k)c_k^\dagger c_k + \epsilon_h d^\dagger d \]  \hspace{1cm} (22)

\[ V = \frac{1}{L} \sum_{k,q} V_{q}c_{k+q}^\dagger c_k d^\dagger d \]  \hspace{1cm} (23)

where \( c_k^\dagger \) creates a conduction electron with energy \( \epsilon(k) \) and \( d^\dagger \) creates a core electron with binding energy \( \epsilon_h \). In higher dimensions \( \{k, q\} \) are vectors \( \{\vec{k}, \vec{q}\} \). Spin indices have been suppressed for compactness. We make the usual assumption that lineshape for the core level measured in an XPS experiment is proportional to the Fourier Transform of the (retarded) core hole Green’s function

\[ G_h(t) = -i\theta(t)|\langle d^\dagger(t)d \rangle| \]  \hspace{1cm} (24)

broadened by an appropriate factor to allow for experimental resolution. In practice to extract a usable lineshape allowance must also be made for the finite lifetime of the core hole (modeled as a Lorentzian with width set by Auger decay processes) and in some cases a symmetric (gaussian) broadening of the line due to interaction with phonons. These issues are discussed in the associated literature [30].

An important many body effect comes into play in the evaluation of this correlation function. As originally observed by Anderson [31], the ground states of a free electron system with and without the impurity are orthogonal, their overlap vanishing as \( 1/N^{\alpha_0} \), where

\[ \alpha_0 = \frac{1}{2} \sum_l \left( \frac{\delta_l}{\pi} \right)^2 \]  \hspace{1cm} (25)

\( N \) is the total number of particles and \( \delta_l \) is the phase shift in the \( l \)-th scattering channel. In three dimensions \( l \) has the natural interpretation of an angular momentum quantum number for scattering states.

In metallic systems this orthogonality makes itself felt in XPS line asymmetries and in a contribution to the FES in X–Ray absorption; the number of zero energy particle hole pairs which may be made at the Fermi edge is essentially only bounded by the level spacing of the system, which in the thermodynamic limit, for a \( d \)-dimensional system in volume \( L^d \) vanishes as \( 1/L \). An important consequence of this for XPS is that in removing a core electron from a metal, a very large number of conduction band electron–hole pairs are excited by the unscreened core hole. This converts the lineshape measured by and core hole photoemission experiment from a simple \( \delta \) functional form

\[ G_h(\omega) \propto \delta(\omega - \omega_T) \]  \hspace{1cm} (26)
to a power law asymmetry

\[ G_h(\omega) \propto \frac{1}{(\omega - \omega_T)^{1-\alpha}} \]  

(27)

where \( \omega_T \) and \( \omega'_T \) are the threshold energies for emission of a core electron (naively given by \( \epsilon_h \)).

For free electrons the XPS exponent \( \alpha \) differs simply by a factor of two from the orthogonality exponent for the overlap \( \alpha_0 \) defined by Anderson. Within the Born approximation, \( \delta_i \) will be proportional to the modulus of the matrix element for the core hole potential in that channel: \( \delta_i \approx |V_i|/v_f \). In one dimension there are only two scattering channels “forward” \( (q \approx 0) \) and “backward” \( (q \approx 2k_f) \), so,

\[ \alpha^{BA} = n_0^2(|V_0|^2 + |V_{2k_f}|^2) \]  

(28)

where \( n_0 = 1/2\pi v_f \) is the density of states at the Fermi surface.

X–Ray spectroscopy of this type is a probe of the low energy charge excitations at a given lattice site, and as such essentially measures its local dielectric constant. We can in fact generalize the result Eq. (28) to an arbitrary many electron system, using the relation

\[ \alpha = \lim_{\omega \to 0} \sum_q |V_q|^2 \frac{\Re\{\chi_{\rho}(q,\omega)\}}{\omega} \]  

(29)

which we derive in Appendix C, provided that certain conditions on \( \chi_{\rho}(q,\omega) \) and \( V_q \) hold.

There is also a closely related shift in the XPS line position

\[ \Delta E = \sum_q |V_q|^2 \Re\{\chi_{\rho}(q,0)\} \]  

(30)

Both of these parameters acquire temperature dependence in a system where the charge susceptibility changes with temperature.

Returning to the case in point — (TaSe\(_4\))\(_2\)I— since the density of states at the Fermi energy is zero in a mean field charge density wave state, and strongly suppressed for an LRA Liquid Eq. (10), we clearly expect very little asymmetry in XPS spectra for (TaSe\(_4\))\(_2\)I in either its metallic or conducting phase. Such asymmetry as exists would follow the form in Figure 7.

The temperature evolution of \( \Delta E(T) \) may well be measurable. However since processes at all energy scales contribute to the real part of the local susceptibility, and the absolute value of the shift is cutoff-dependent there is no simple universal formula for the shift valid at all temperatures. The temperature dependence of a relative line shift must be found numerically. Results for this quantity are plotted for our parameterization of the model in Figure 7.

This lack of asymmetry is to be expected: many body effects related to the existence of a Fermi surface will not occur in a system with a gap (or quasigap). However, such
an argument can only be applied in a system where the quasi–particles are in some sense electron—like. It is clearly unreliable in the case of a Luttinger Liquid where the quasi–particles are stable but are not electron–like in character. We consider this case below.

The X–ray response of strongly correlated one dimensional metal (a Luttinger Liquid) has become something of a cause célèbre in recent years. “Forward scattering” from a core level may easily be treated within the bosonization scheme used to diagonalize the interacting problem, leading to a suppression (enhancement) of the asymmetry measured in a system with repulsive (attractive) interaction between electrons, compared with that measured for non–interacting electrons [32].

In Appendix E we present an exact solution of the forward scattering contribution to XPS in a Luttinger liquid; here we simply reproduce the result in convenient form

$$\alpha_{BA}^f (V) = K_\rho \rho v \rho^2 \alpha_{BA} f$$

where $\rho_\rho$ and $K_\rho$ are the parameters of the charge sector of the LL, defined in Equation (13), and $\alpha_{BA} f$ is the result for non interacting electrons within the Born Approximation.

Unfortunately “backward scattering” introduces terms nonlinear in bose fields into the Hamiltonian and make the problem very much harder to treat analytically. Renormalization group analysis in fact suggests that strength of this nonlinear term flows to infinity, “breaking” the one–dimensional chain of atoms [25]. Within this “open chain” interpretation of the RG results, the contribution to the orthogonality exponent $\alpha_O$ from backward scattering is expected to take on the universal value of 1/16, and the orthogonality exponent has the value

$$\alpha_O = \frac{1}{2} \left( \frac{\delta_f}{\pi} \right)^2 + \frac{1}{16}.$$  

This result may be derived very elegantly from the use of boundary conformal field theory [33].

Equivalent results for XPS response have been derived in expansions about the “open chain” fixed point [34]. Generically these predict an exponent

$$\alpha_E = 2K_\rho \rho v \rho^2 \alpha_{BA} f + \frac{1}{8}$$

at threshold, with a crossover to a different non–universal scaling law at a finite energy determined by the strength of the core–hole conduction electron coupling. A particularly elegant approach to the XPS problem which reproduces these and many other standard results is provided by the use of boundary conformal field theory [33].

It should also be noted that not all authors have found their results in agreement with the “open chain” interpretation set out above, with one asserting that backward
scattering terms can lead to an enhancement of the FES \[35\]. A recent numerical treatment of the problem with references to earlier analytical work is provided by \[36\].

No predictions have yet been made for the temperature dependence of the XPS exponent in a LL, but we can speculate that these will also obey non–integer power laws controlled by \(K_\rho\). As stated above XPS measures the leading \(\omega\) dependence of the local charge susceptibility a system. For a LL, we may divide the susceptibility into a regular part at \(\chi_\rho(q \approx 0)\) and an anomalous part at \(\tilde{\chi}_\rho(q \approx 2k_f)\). The former has the same structure as in a free electron gas (up to charge velocities); from scaling arguments we anticipate that the temperature dependence of the latter will be a power law controlled by the interaction parameter \(K_\rho\).

As stressed above, XPS is a zero energy probe and the scaling of \(\tilde{\chi}_\rho\) will be cut off by any gap.

Core level studies for materials with a charge density wave groundstate (see, e. g., Ref. \[37\]) usually reveal gross differences between spectra taken above and below the transition temperature. There are two fundamental reasons for these differences – the change in the local environment of core states due to a structural transition or charge density wave, and changes in the charge susceptibility induced by the charge density wave transition, which modify the lineshape and position, as discussed above.

In a one–dimensional tetramerized charge density wave state (assuming perfect commensurability) there are two inequivalent sites in each unit cell. The unbalanced charge accumulated due to the charge density wave will be different at each of these sites leading to a splitting in the XPS lines proportional to the magnitude of the charge density wave \(\langle \rho(2k_f,T) \rangle\), and therefore following it in temperature dependence. It is unlikely that such a splitting would be observed in an incommensurate charge density wave system like \((TaSe_4)_2I\) although this has been a subject of some contention \[38\].

Incommensurability can be expected to lead to the smearing of the core level threshold energy over a range of energies again proportional to the magnitude of the charge density wave, and therefore to lines whose width follows \(\langle \rho(2k_f,T) \rangle\). In the quasi–static picture on which our model is based on the splitting (or smearing) of the core line observed in the ordered phase would persist into the conducting phase, since the structural deformations of the lattice persist — the loss of order is a loss of three–dimensional coherence only and is essentially irrelevant to the site–local physics of core holes.

Importantly however, a splitting (smearing) of the line due to the inequivalence of \(Ta\) sites will not alter the asymmetry of the underlying lineshape. If there are zero energy charge excitations in the conducting phase the measured split (smeared) lineshape should also be asymmetric. Shifts in the line due to changes in the local susceptibility will persist for the same reason. In bulk \(Ta\) the 4\(f\) orbitals may be fitted with a Doniach–Sunjić lineshape and has an asymmetry \(\alpha_E \sim 0.1\).
There are a number of other effects which need to be borne in mind. Foremost among these is spin–orbit coupling which can split core lines by large energies. In the case of the \( Ta_{4f} \) state discussed above spin–orbit coupling leads to a splitting of \( \sim 3eV \) between \( 4f_7/2 \) and \( 4f_5/2 \) states.

We should also be aware that an attractive potential (such as a core hole) in a one dimensional electron system will generally have a bound state. The presence of this bound state will modify the threshold for photoemission out of the core level (giving in general two thresholds, one for sites with the bound state filled and one for those where it is empty) and, in a truly metallic system, will also modify the asymmetry measured in each of these cases \cite{39}. As splitting due to bound states will be uncorrelated with the lattice distortion, it can in principle be distinguished from one due to inequivalent sites in a distorted lattice. The possibility of a line split by a bound state appearing as a single (asymmetric) line in XPS carried out at finite resolution poses a more serious threat to the interpretation of data on these systems, and would need to be considered before very strong conclusions were drawn about any measured asymmetry.

8. NMR

NMR provides a local probe of spin excitations which is exactly complementary to XPS (a probe of local charge excitations). In fact, up to a structure factor \( F(q) \), the nuclear relaxation rate \( 1/T_1 \) is given by precisely the same formula as we derived in \text{Appendix D} for the XPS asymmetry, but with the \text{spin} susceptibility \( \chi_\sigma \) substituted for the \text{charge} susceptibility \( \chi_\rho \) and the structure factor \( F(q) \) substituted for the core–hole conduction electron interaction matrix element \( |V_q|^2 \).

\[
\frac{1}{T_1 k_B T} = \frac{\gamma^2}{2 \mu_B^2} \lim_{\omega \to 0} \sum_q F(q) \frac{\Im \{ \chi_\sigma(q, \omega) \} \omega}{\omega}.
\]

(34)

Here \( \mu_B \) is the Bohr magneton and the nuclear spin has gyromagnetic ratio \( \gamma \). We shall assume purely on-site coupling. This leads to a momentum-independent coupling \( F \).

Then the rate is simply proportional to the slope of the absorptive part of the local spin susceptibility at very low frequencies. We shall neglect spin-orbit coupling so that the spin susceptibility is well-defined and isotropic.

Since the single-particle Green’s function for the LRA liquid is diagonal in spin indices, we may evaluate the spin susceptibility in terms of the density of states in the same way as we evaluate the charge susceptibility in \text{Appendix D} to find

\[
\frac{1}{T_1 k_B T} = 2 \pi \gamma^2 k_B F n_0^2.
\]

(35)

where \( n_0 \) is the density of states at the Fermi energy. For a regular metal (Fermi Liquid) where \( n_0 \) is not a function of temperature this gives a constant relaxation rate (Korringa Law).
The quantity $n^2_0$ is however very strongly temperature dependent in the LRA theory (Figure 6) and so the temperature dependences of the relaxation rate and can be used directly to measure of the extent to which the pseudogap depresses the density of states at the Fermi energy. NMR measurements are in principle possible for $(\text{TaSe}_4)_2\text{I}$ since $\text{Se}$ at least is NMR active, but no data at present exist.

The NMR Knight shift is determined not by the local, but by the uniform susceptibility

$$\frac{\Delta H}{H_0} \sim \chi_\sigma$$

and so follows this in temperature dependence. This is plotted in Figure 3 for our paramatrization of the LRA model.

In a LL, the temperature dependence of $1/T_1T$ is dominated at low temperatures by the scaling dimension of the $q \sim 2k_f$ part of the spin susceptibility, which is set by the anomalous dimension of the charge field $K_\rho$

$$\frac{1}{T_1T} \sim 1 + \left( \frac{T_0}{T} \right)^{1-K_\rho}.$$  \hfill (37)

where $T_0$ is the characteristic temperature at which the $q \sim 0$ and $q \sim 2k_f$ susceptibilities are of equal size.

Data for the quasi one-dimensional organic spin density wave (SDW) system $(\text{TMTSF})_2\text{ClO}_4$ have been interpreted as showing LL behaviour over a range of temperatures just above the SDW transition temperature, with the rather small value of $K_\rho \sim 0.15$ \[40\] found from a fit to $1/T_1T$. As far as we are aware no such analysis of NMR data has been attempted for a CDW system.

9. Comparison with other Theories

We have presented predictions for XPS and NMR. This has a particular goal. In a theory such as the LRA model the pseudogap is felt equally in both spin and charge channels, and should be evident in the suppression of both XPS asymmetry and nuclear spin relaxation. Importantly, both are local probes of the charge(spin) susceptibility and as such, directly comparable.

In the limit of large coherence length the LRA spectral function (7) reduces to the sum of two lorentzians. In the language of many–body Green’s functions we may say that the poles associated with fermionic quasi–particle excitations have migrated from the real axis into the complex plane, becoming purely imaginary for zero frequency. The fact there are still simple poles in the electron Green’s function means that these quasiparticle excitations are electron–like in nature and therefore carry both spin and charge. If the effects of the mean field gap persist in the spin channel for the metallic
phase, they will also persist in the charge channel, and the (quasi–)gaps measured in each channel should have the same temperature dependence — in the language associated with high-temperature superconductivity, the “quasi–gap” and the “spin–gap” should be in exact correspondence.

We can make this statement more formal by considering the ratios of the XPS asymmetry and the NMR relaxation time

\[ R = \frac{\alpha(T)}{1/T_1T} \]  

(38)

Within the LRA model (or any other model in which the pseudogap is felt equally in spin and charge channels) \( R \) should be essentially temperature–independent.

Almost none of these features are shared with the canonical one–dimensional model of interacting electrons which we may most meaningfully compare with experiments on \((\text{TaSe}_4)_2\text{I}\) (and other quasi one-dimensional charge density wavesystems) — the Luther-Emery (LE) model. Here there are no fermionic quasiparticles and the gap exists uniquely in the spin excitations of the system. This means that the ratio \( R \) of Equation (38) should be very strongly temperature dependent, due to the activated behavior of spin excitations.

A plausible form for the spectral function of the LE liquid capturing the essential features of the gap in spin excitations the has been proposed by Voit [41]. The spectral function has two dispersing maxima, one associated with charge and the other with spin excitations, but now only the spin peak is a true singularity; the divergence at the charge peak is cut off by the spin gap.

The spectral properties of a related field–theoretical model of electrons interacting with phonons in one–dimension have also been derived by Wiegmann [42]. This goes somewhat beyond the considerations of the other theories alluded to in this article in identifying the readjustment of the order parameter which accompanies the introduction or removal of an individual electron. It is characterized by extremely broad and asymmetric dispersing features, even in the absence of electron–electron interaction. The extreme breadth of the dispersing features in this model resembles photoemission spectra taken on the high-\(T_c\) cuprates rather more than those taken on quasi one–dimensional conductors.

Because of the broadness and asymmetry of features in the LE spectral functions and its dual peak structure, it would be difficult to extract a single energy scale from it empirically. An experimental spectrum taken at finite resolution might well “measure” a different gap scale and temperature dependence different from that determined by transport, optical conductivity, or susceptibility experiments.

Thus the LRA model offers a better description of existing photoemission data for this system [4]. The LE model may prove to be more nearly applicable to the other most commonly studied inorganic quasi one-dimensional charge density wave system,
Blue Bronze \((KMnO_3)\), but faces some challenge in explaining the suppression of charge excitations over the energy range \(0.1 \rightarrow 0.3\text{eV}\) seen in optical conductivity.

10. The gap discrepancy

There remains the discrepancy in gap values mentioned at the outset.

First note that only the photoemission value is truly out of line. Based on this we may put forward three speculative resolutions.

One is that photoemission, which takes place on a very fast time scale and is a high energy process which may couple to many excitations besides the formation of a hole, cannot be compared directly with a long–time scale, low energy experiment such as transport. This point of view is broadly compatible with the treatment of the electron–phonon problem performed by Brazovskii and Dzyaloshinskii \([43]\) in which there is a clear separation of time scales between different electron and phonon excitations of the system.

Second, a movement of intensity away from the Fermi energy in photoemission spectra could originate in “extrinsic” energy loss processes, i. e. , those affecting the outgoing electron. In the range considered, Drude and phonon losses are the most important loss mechanisms. These extrinsic processes may be independently measured by electron loss spectroscopy \([47]\).

Third, midgap states may explain the mismatch between photoemission and transport gaps. These are highly localized states in the middle of the gap, which cannot carry a current and (due to their small number) have a small cross section for photoemission, but which offer a reservoir of charge that can be thermally excited over (half) the gap and participate in transport. This conjecture leads directly to the prediction that the activation energy measured at low temperatures is of order \(\Delta\) and not \(2\Delta\). The transport activation energy is indeed approximately half the gap measured in photoemission, and a possible mechanism for the generation of localized mid–gap states does exist in \((TaSe_4)_2I\) through interaction with the lattice distortion. There are four equivalent ways of accomplishing the nearly commensurate tetramerization of the lattice which is observed experimentally, and it is natural to suppose that this “frozen” phonon is divided into domains with different phase by kinks (solitons) in the order parameter. That kinks in an order parameter can bind (fractional) charge is well known and has been extensively studied in the case of polyacetylene \([44]\), which has a half filled band. A numerical study of the formation of mid–gap states in the nearly commensurate quarter–filled case was performed by Machida and Nakano \([45]\), who find fractal structure in the density of states reminiscent of the Hofstader problem \([46]\); in fact both the motion of an electron in an incommensurate potential in one dimension and in a magnetic field at incommensurate Landau level can be described by the same almost Mathieu equation.
As we have been arguing that the lattice distortion persists in the normal state of (TaSe$_4$)$_2$I (a weak superlattice corresponding to the condensed TA Phonon mode is still visible in X–Ray experiments at 300K) we can further speculate that the midgap states will persist to these temperatures, leading to the observation of the smaller “gap” in room temperature optical conductivity. However, this hypothesis has the weakness that the states involved must have sufficient weight to dominate transport properties but not enough to show up in photoemission.

Note that tunneling experiments on (TaSe$_4$)$_2$I would be extremely informative. This experiment also measures the density of states. Given that photoemission is in conflict with other data, a check is necessary.

Thus the different gap sizes measured by different probes in quasi–one dimensional systems are hard to reconcile with the LRA model unless some additional mechanism is postulated a posteri to explain the discrepancy. They may be somewhat less surprising within a strong interaction scenario, but the different determination of (pseudo–)gap sizes and temperature dependence by different probes is not a problem of the exotic non–Fermi liquid conducting phase only, but one which needs to be addressed also in the context of the ordered phase. In the metallic phase however, XPS provides, at least in principle, a novel means of exploring whether (quasi–)gaps exist for both spin and charge excitations or only for spin, and might be particularly informative if taken in conjunction with NMR experiments.

11. Comparison with Underdoped High-temperature Superconductors

What light does (TaSe$_4$)$_2$I shed on the pseudogap in high-$T_c$ superconductors? Photoemission results on the two systems are the obvious place to start. In underdoped Bi$_2$Sr$_2$CaCu$_2$O$_{8+x}$ above $T_c$ the peak of the spectral function $A(\vec{k}, \omega)$ never reaches the Fermi energy, stopping about $\sim 10$meV below the Fermi energy when $\vec{k}$ is along the $(0, \pi)$ direction [48]. This precise size of this pseudogap depends on doping and temperature and vanishes at a temperature $T^* > T_c$. This observation is qualitatively similar to that in (TaSe$_4$)$_2$I. There is, however, more than an order of magnitude difference in the size of the pseudogaps. Furthermore, the pseudogap in Bi$_2$Sr$_2$CaCu$_2$O$_{8+x}$ is anisotropic with little or no pseudogap observed in the $(\pi, \pi)$ direction. This possibility does not arise in (TaSe$_4$)$_2$I. The similarities go beyond this. The uniform magnetic susceptibility is suppressed in underdoped high-$T_c$ systems [19] and in (TaSe$_4$)$_2$I [5], showing that the pseudogap is present in the spin channel as well. The temperature dependence of the resistivities $\rho(T)$ is superficially very different. In the underdoped high-$T_c$ systems, $\rho$ rises rapidly and monotonically between $T_c$ and $T^*$, though there are strong deviations from the linear behavior of $\rho(T)$ which is characteristic of the optimally doped material. In (TaSe$_4$)$_2$I, $\rho$ is roughly independent
of temperature in experiments, as we have seen. However, this may only reflect the fact that the accessible regime of temperatures does not reach up to $T_{MF}$. We would expect $\rho$ to rise when $T \sim T_{MF}$, as seen in Fig. 1. Finally, we may compare optical conductivities $\sigma(\omega)$. The most interesting high-$T_c$ data from our point of view are actually $c$-axis conductivities which have no Drude peak at low frequencies. These show a very clear pseudogap opening up as a function of temperature. In the $a$-$b$ plane conductivity there is a Drude peak. This interacts in a subtle way with the suppression of the density of states and the evolution of the electron lifetime due to the pseudogap, rendering the interpretation of the data somewhat complicated. In (TaSe$_4$)$_2$I we are more fortunate in that the Drude width is considerably less than the pseudogap energy and the structures in $\sigma(\omega)$ are therefore well separated. Again, given the difference in parameters, it appears that the two systems are rather comparable. NMR and tunneling also show evidence for a pseudogap in underdoped high-$T_c$ systems. These experiments have not been performed in (TaSe$_4$)$_2$I, but would be illuminating, as we have already stressed.

The very strong similarity between the two systems suggests a common origin for the pseudogap behavior. In (TaSe$_4$)$_2$I, it is clear that the properties of the pseudogap phase are essentially determined by the fluctuations remaining from the low-temperature phase. There is a very large difference between the actual critical temperature and the mean-field temperature. This is expected in this quasi-one-dimensional material. In the high-$T_c$ systems, the difference is not so large, as the system is quasi-two-dimensional. If we take into account this dissimilarity it appears that in the intermediate pseudogap region, the fluctuations from the ordered phase are the determining factor. Thus, the comparison supports the point of view that the origin of the pseudogap in is superconducting fluctuations. The anisotropy in the pseudogap is consistent with this as well.

Spin–charge separated theories of the pseudogap regime of high-$T_c$ superconductors analogous to the LE liquid have been advanced by several authors. The comparison of XPS and NMR data for these systems along the lines which we suggested for a one-dimensional charge density wave system might also shed light on whether the (pseudo-)gap exists in both spin and charge channels. We hope to develop this idea further in a later paper.

12. Conclusions

The Lee, Rice and Anderson model offers the simplest possible scenario for fluctuations of charge density wave order in quasi one-dimensional charge density wave systems that reduces simply to the mean field ordered state. The naive application of this model to existing data for the quasi one-dimensional charge density wave system (TaSe$_4$)$_2$I is
quite successful. In those cases where the LRA model fails to explain experimental data for this system above the charge density wave transition temperature ($T_{3D}$), the usual mean field picture of the ordered state must also be called into question below $T_{3D}$. The most important of these discrepancies is the size of the charge density wave gap (pseudogap) which is found to be of different size by different experimental techniques, both above and below $T_{3D}$.

This simple view of the origin of a pseudogap in a quasi–one–dimensional system should be contrasted with the canonical picture of “gapping” in 1–D, strongly correlated systems with strong CDW fluctuations, in which non–current conserving terms in the Hamiltonian lead to the formation of a gap for spin, but not for charge excitations. In this scenario, dispersing features in the electronic spectral function are generally extremely broad and asymmetric, and while the ordered state of the system must be three-dimensional, it need not be mean field like in nature. In those cases where we have been able to compare the LRA model directly to experiments on (TaSe$_4$)$_2$I it seems to offer a better description of data than existing predictions for strongly correlated models.

XPS provides, at least in principle, a novel means of exploring which of these scenarios is correct, and might be particularly informative if taken in conjunction with NMR experiments. Tunneling measurements of the density of states would serve as a useful check on photoemission.

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Since completing this work we have learned of a calculation of the intrinsic conductivity of the LRA liquid in the memory–function formalism by Voit [preprint cond-mat/9711064, to be published in Proc. Ninth Int. Conf. on Recent Progress in Many Body Theories (Sydney), ed. D Nielson, World Scientific]. His result of $\sigma_0 \sim \langle \psi^2(T) \rangle \xi(T)$ also represents a weakly temperature dependent and monotonically increasing conductivity.

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**Figure captions**

**Figure 1.** a) Structure of Ta chains in (TaSe₄)₂I. b) Schematic displacement of Ta atoms in tetramerized ground state.

**Figure 2.** Example of ARPES spectrum for dispersing feature with $k=k_F$ and theoretical fit, taken from Ref. 4.

**Figure 3.** The temperature dependence of the uniform susceptibility as a function of temperature. The points are data and the line is the LRA model fit, both from Ref. 5.

**Figure 4.** The DC resistivity over the experimentally accessible temperature range. The data in (a) are taken from Ref. 12 and the theoretical curve in (b) is plotted using Eq. 8.
**Figure 5.** a) Experimental spectra for the optical conductivity \((\text{TaSe}_4)_2\text{I}\) taken from Ref. 8. b) The intrinsic optical conductivity of an LRA liquid as calculated from current–current correlations according to Eq. 12.

**Figure 6.** The temperature dependence of the density of states at the Fermi energy squared normalized to free electron values, for the LRA model, as parametrized to describe optical conductivity measurements. The temperature dependence of NMR \(1/T_1\) and the XPS asymmetry \(\alpha_E\), should both follow up to the accuracy of this parametrization of the model.

**Figure 7.** Numerically determined change in the local static susceptibility \(\sum_q \chi(q,0,T)\) relative to \(T_{3D}\). This determines the shift in XPS lines.

**Figure 8.** a) MF theory of the charge density wave state in terms of multiple scatterings between right and left moving electron states. These may be resummed to give a self energy correction which coincidently is equivalent to b) the first term in a perturbation theory developed using the \(\omega \to 0\) limit of the phonon propagator \(D(q) \sim \delta_{q \pm 2k_F} \delta(\omega)\).

**Figure 9.** Diagrams which must be evaluated when using the \(\omega \to 0\) limit of the phonon propagator, as in the theories due to Sadovskii. Propagators may be modified to take account of the finite correlation length of the lattice distortion, but the theory is then no longer exactly soluble. Crossing diagrams at higher order are included.

**Figure 10.** Diagrams calculated in the “static non–crossing “ approximation with the phonon propagator is \(\delta_{q \pm 2k_F} \delta(\omega)\).
Appendix A. Formal standing of the LRA theory

In this appendix we discuss the nature and validity of the LRA theory from a technical rather than phenomenological point of view.

We begin by rederiving the self energy correction (6) using equations of motion in the spirit of the original LRA paper, but showing that on a more careful examination of the nature of the averaging involved, the equations of motion do in fact close.

Our starting point is the Hamiltonian

$$H_{LRA} = \sum_k \epsilon(k)c_k^\dagger c_k + \sum_{Q,k'\geq 0} \left[ \Psi_Q^\ast c_{k' - Q}^\dagger c_k + \Psi_Q c_{-k' + Q}^\dagger c_{-k'} \right]$$ (A1)

$$\Psi_Q = \frac{1}{\sqrt{L}} g(Q) \langle u(Q) \rangle.$$ (A2)

and

The imaginary time dependence of the single electron Green’s operator (in the Heisenberg picture) is given by

$$\hat{G}(k',k,\tau) = -T\delta(\tau) c_{k'}(0)$$ (A3)

$$= -\{ \Theta(\tau)c_{k'}(\tau)c_k^\dagger(0) - \Theta(-\tau)c_k^\dagger(0)c_{k'}(\tau) \}$$ (A4)

and its evolution follows

$$\frac{\partial \hat{G}(k',k,\tau)}{\partial \tau} = -\delta(\tau)\{c_{k'}(0),c_k^\dagger(0)\} - T\frac{\partial c_{k'}(\tau)}{\partial \tau} c_k^\dagger(0).$$ (A5)

The Fermi field in turn has dynamics governed by

$$c_{k'}(\tau) = e^{H\tau} c_{k'} e^{-H\tau}$$ (A6)

$$\frac{\partial c_{k'}(\tau)}{\partial \tau} = e^{H\tau}[H,c_{k'}] e^{-H\tau}$$ (A7)

and the phonon field, by explicit assumption, is static — i.e. has no dynamics.

Inserting the Hamiltonian (A1) in (A6) we find

$$\frac{\partial \hat{G}(k',k,\tau)}{\partial \tau} = -\delta(\tau)\delta_{kk'} - \epsilon(k')\hat{G}(k',k,\tau)$$ (A8)

$$- \left\{ \sum_Q \Psi_{Q}^\ast \hat{G}(k + Q,k,\tau) + h.c. \right\}.$$ (A9)

Then for the Green’s operator with $k' = k$.

$$\frac{\partial \hat{G}(k,\tau)}{\partial \tau} = -\delta(\tau) - \epsilon(k)\hat{G}(k,\tau)$$ (A10)

$$- \left\{ \sum_Q \Psi_{Q}^\ast \hat{G}(k + Q,k,\tau) + h.c. \right\}$$ (A11)
We introduce the Fourier transform
\[ \hat{G}(\tau) = \frac{1}{\beta} \sum_{\omega_n} \hat{G}(i\omega_n)e^{-i\omega_n} \]  
(A12)

Whence
\[ -i\omega_n \hat{G}(k, i\omega_n) = -1 - \epsilon(k) \hat{G}(k, i\omega_n) \]
\[- \left\{ \sum_Q \Psi_Q^* \hat{G}(k + Q, k, i\omega_n) + h.c. \right\} \]  
(A13)

Physically we are interested in scattering between the two Fermi points, i.e. \( k' \approx k_f, Q \approx 2k_f \), i.e.
\[ [\epsilon(k) - i\omega_n] \hat{G}(k, i\omega_n) = 1 - \sum_Q \Psi_Q^* \hat{G}(k - Q, k, i\omega_n) \]  
(A14)

Similarly,
\[ [\epsilon(k - Q) - i\omega_n] \hat{G}(k - Q, k, i\omega_n) = - \sum_{Q'} \Psi_{Q'}^* \hat{G}(k + Q' - Q, k, i\omega_n) \]  
(A15)

which implies
\[ [\epsilon(k) - i\omega_n] \hat{G}(k, i\omega_n) = 1 + \sum_{QQ'} \frac{\Psi_{Q'}^* \Psi_Q \hat{G}(k + Q' - Q, k, i\omega_n)}{\epsilon(k - Q) - i\omega_n} \]  
(A16)

We now turn this relationship between operators into an equation for the single electron Green’s function by taking the expectation value of both sides
\[ [\epsilon(k) - i\omega_n] \langle \hat{G}(k, i\omega_n) \rangle = 1 + \sum_{QQ'} \frac{\langle \Psi_{Q'}^* \Psi_Q \rangle \langle \hat{G}(k + Q' - Q, k, i\omega_n) \rangle}{\epsilon(k - Q) - i\omega_n} \]  
(A17)

where \( \langle \ldots \rangle \) denotes both thermal and quantum mechanical averaging.

In the case of the classical field \( \Psi_Q \) quantum averaging is irrelevant and we are left with the thermal average \( \langle \Psi_{Q'}^* \Psi_Q \rangle_T \) over all possible configurations of the static phonon field. By definition \( \langle \langle \hat{G}(k, i\omega_n) \rangle \rangle = G(k, i\omega_n) \) the temperature Green’s function for the system.

We note that for a many–chain system with “frozen” phonon disorder one might equally motivate an ensemble average on potentials from the fact that all experiments measure average over many chains, and the potentials on different chains would in general be different.

Following Scalapino, Sears and Ferrell (SSF) \[35\], LRA consider consider a one–dimensional classical order parameter \( \Psi_Q \) described by a free energy
\[ F[\Psi_Q] = a(T)|\Psi_Q|^2 + b(T)|\Psi_Q|^4 + c(T)(Q - 2k_F)^2|\Psi_Q|^2, \]  
(A19)

where the parameters \( a(T), b(T) \) and \( c(T) \) are taken from the mean field treatment of the electron–phonon interaction. Using this free energy to perform the thermodynamic
average it is then found that correlations of lattice at $2k_F$ order decay exponentially with distance

$$\langle \Psi(x)\Psi(x') \rangle_T = \langle \psi^2(T) \rangle \cos[2k_F(x-x')] \exp[-|x-x'|\xi^{-1}(T)] \quad (A20)$$

where the temperature dependence of the two parameters follows from $\langle \psi^2(T) \rangle$ and $\xi^{-1}(T)$ may be found from an exact mapping onto a quantum mechanical anharmonic oscillator problem [55].

It follows from (A20) that

$$\langle \Psi_Q^* \Psi_Q \rangle_T = \delta_{QQ'} \langle \psi^2(T) \rangle \frac{\xi^{-1}(T)}{\pi} \frac{1}{(Q-2k_f)^2 + \xi^{-2}(T)} \quad (A21)$$

and the equations of motion now close. We assume that within this thermal ensemble $\langle \Psi_Q \rangle = 0$ which implies that there is no anomalous propagator above the three-dimensional ordering temperature $T_{3D}$.

The remaining sum over $Q$ is performed as a contour integral, using the result that, for linearized dispersion

$$\epsilon(k-2k_f) = -\epsilon(k) \quad (A22)$$

yielding

$$G(k, i\omega_n)^{-1} = i\omega_n - \epsilon(k) - \frac{\langle \psi^2(T) \rangle}{i\omega_n + \epsilon(k) \pm iv_f \xi^{-1}(T)} \quad (A23)$$

with the choice of sign depending on the half plane to which the function is to be continued.

The self–energy correction which we derived above

$$\Sigma_{LRA}(k, i\omega_n) = -\frac{\langle \psi^2(T) \rangle}{i\omega_n + \epsilon(k) \pm iv_f \xi^{-1}(T)} \quad (A24)$$

has the correct limits for $\xi^{-1}(T) \to 0$ (BCS mean field theory with gap $\Delta^2 = \langle \psi^2(T) \rangle$) and for $\langle \psi^2(T) \rangle \to 0$ (free electron gas). Physically it can be thought of as describing the pairing of a coherent electron of momentum $k \approx k_f$ with an incoherent hole of momentum $k \approx -k_f$. However since it at first sight a somewhat crude theory, our use of it requires some clarification and justification.

The physical motivation is clear – below the mean field transition temperature there is a very strong separation of time scales between the soft phonon modes and the electrons. This observation might equally inspire us to develop a perturbation theory for electron–phonon coupling in which the electrons scattered elastically from the fluctuations of lattice order. This would require using the full electron–phonon vertex of the Fröhlich Hamiltonian (1) and the $\omega \to 0$ limit of the phonon propagator.
Indeed if we interpret the result of the thermal average over static phonon fields \( A_21 \) as an \( \omega \to 0 \) phonon propagator

\[
D(Q) = \langle \psi^2(T) \rangle \frac{\xi^{-1}(T)}{\pi} \frac{1}{(Q - 2k_f)^2 + \xi^{-2}} \tag{A25}
\]

then the lowest order self energy correction for electrons scattering off this (quantum mechanical) phonon field is indeed the LRA result (A24), and the LRA theory is often discussed in these terms.

It is not hard to calculate the corrections to this self–energy which occur at the next (and higher) order in this interaction \[56\]. They are not small, and tend to “wash out” the pseudogap found in the LRA theory — why then should we trust it?

Under the model assumptions made above about the thermal ensemble of lattice potentials, the equations of motion for the Hamiltonian (4) close. This means that the LRA theory we present is the correct solution of a slightly different problem. We explain why, and what this problem is, below.

By using the expectation value of the phonon field in the Hamiltonian (4) we are going somewhat further than taking the \( \omega \to 0 \) limit of a quantum mechanical problem; we are removing the phonons from the quantum mechanics of the problem entirely. The “frozen” lattice is treated strictly as a static external field – a classical object.

This approach has the great advantage of reducing exactly to the familiar “mean field” case in the fully ordered limit where

\[
\Psi_Q = \Delta \delta_{Q \pm 2k_F}. \tag{A26}
\]

in which case the Hamiltonian is

\[
H = \sum_k \epsilon(k) c_k^\dagger c_k + \sum_k [\Delta^* c_{k-2k_F}^\dagger c_k + \Delta c_{-k+2k_F}^\dagger c_{-k}] \tag{A27}
\]

\[
\Delta = \frac{1}{\sqrt{L}} g(2k_F) \langle u_{2k_F} \rangle. \tag{A28}
\]

This familiar Hamiltonian may be solved exactly by the equation of motion technique used above, or by canonical transformation, and one obtains a self–energy of the form

\[
\Sigma_{MF}(k, i\omega_n) = \frac{\vert \Delta \vert^2}{i\omega_n + \epsilon(k)} \tag{A29}
\]

The same self–energy correction is indeed the result found in a perturbation theory for electrons interacting with a \( \lim \omega \to 0 \) phonon propagator

\[
D(Q) = \Delta \delta_{Q \pm 2k_f} \delta(\omega) \tag{A30}
\]

but only at lowest order. Resumation of the remaining diagrams at higher order \[26\] does not lead to recovery of the correct BCS–like mean field form for the electron Green’s function. Instead one finds a propagator for a system with a distribution of real gaps.

\[
G(k, i\omega_n) = \int_0^\infty dx e^{-x} \frac{i\omega_n}{i\omega_n^2 - \epsilon_k^2 - x\Delta^2} \tag{A31}
\]
a result that first published by Sadovskii [57]. A later attempt by Sadovskii [58] to
generalize this treatment to the case with a finite coherence length (phonon propagator
A25) has been widely discussed but seems to be flawed [59].

The reason for the apparent contradiction between the exact result and this
resumation of perturbation theory is that so far as Hamiltonian (A27) is concerned,
the wrong perturbation theory has been resummed. The topology of the diagrams for
scattering off an external field (in our case “frozen” phonons) and for scattering from
an $\omega \to 0$ phonon propagator are different because a propagator (two points joined
by a line) explicitly correlates pairs of scattering events, whilst all scatterings from an
external field are independent of one another.

In solving the mean field Hamiltonian we have, in diagrammatic language, resummed
the infinite series of all possible multiple scatterings which transfer electrons between the
two Fermi points (see Equation (8)). The vertex in (A27) is of the form of an external
field which scatters particles from the right Fermi point to the left (or vice versa) whilst
preserving the new momentum $q$.

If one wishes do perturbation theory starting from the Hamiltonian one should
consider diagrams of the same type, for the same reason. The coincidence between the
first order self energy correction a perturbation theory developed using an $\omega \to 0$ phonon
propagator with Lorentzian form and the LRA self energy is in some sense just that
– a coincidence – and moreover the same coincidence as the correspondence between
the exact self energy of the usual mean field picture and the lowest order self–energy
correction for interaction with a phonon propagator of delta function form.

Our goal is to understand the effects of fluctuations of charge density wave order in
a quasi–one dimensional system. In the absence of any exact solution to which we can
compare, whether it is a better approximation scheme to remove quantum mechanics
from the phonon field altogether and so be able to recover mean field theory, or to
consider a problem in which both electrons and phonons are quantum mechanical objects
but scattering between them is elastic remains an empirical question. As the thermal
averaging over static field configurations in the LRA scheme in some ways imitates the
averaging over many chains which must take place in the real system, even an exact
solution which called the LRA scheme into question in 1D might not invalidate its
application to real systems.

A comprehensive treatment of the Sadovskii model and related technical issues is
supplied by Tchernyshyov [59]. A slightly different approach to the same problem has
also been considered by Millis and Monien [60].
Appendix B. Parametrization of Model

The parametrization of the model involves determining the temperature dependance of the two parameters of the self energy correction, \( \langle \psi^2(T) \rangle \) and the coherence length \( \xi^{-1}(T) \). This is to some extent arbitrary. As we intend to use the model in a phenomenological but self–consistent way they should ideally be taken from experiment; in order to have a simple working picture we borrow the analysis presented in the original LRA paper which leans heavily on the results of SSF [55].

The classical field \( \Psi_Q \) has a free energy with parameters taken from the mean field (linear response) perturbative treatment of the 1D Fröhlich Hamiltonian:

\[
F[\Psi_Q] = a(T)|\Psi_Q|^2 + b(T)|\Psi_Q|^4 + c(T)(Q - 2k_F)^2|\Psi_Q|^2, \tag{B32}
\]

with

\[
a(T) = D_0 \frac{T - T_c}{T},
\]

\[
b(T) = D_0[b_0 + (b_0 - b_1)\frac{T}{T_c}],
\]

and

\[
c(T) = D_0\xi_0^2(T),
\]

where \( D_0 \) is the (constant) density of states for the band, which is taken to have width \( 2\epsilon_F \). The parameter \( \xi_0(T) \) is the length scale emerging naturally from the linear response analysis of the one–dimensional electron phonon problem

\[
\xi_0(T) = \frac{4\pi k_B T}{\sqrt{7}\zeta(3)h\nu_f} \tag{B33}
\]

We fix \( b_0 \) and \( b_1 \) to give the correct zero temperature value of the gap \( \Delta_0 \) for the experiment under consideration (\( \Delta_0^{ARPES} \neq \Delta_0^{TRANSPORT} \)) according to

\[
b_0 = \frac{1}{2\Delta_0^2}, \tag{B34}
\]

and

\[
b_1 = \frac{7\zeta(3)(1.76)^2}{16\pi} \frac{0.5}{0.5}.
\]

The problem of determining \( \langle \psi^2(T) \rangle \) and \( \xi^{-1}(T) \) then reduces to that of finding the low lying energy levels of a particle moving in an anharmonic potential well, the shape of which is determined by the coefficients of the free energy

\[
H = -\frac{1}{4}\frac{k_B T_c^2}{D_0} \frac{\partial^2 \Psi}{\partial x^2} + a(T)|\Psi|^2 + b(T)|\Psi|^4 \tag{B35}
\]
This problem may be solved numerically, or approximately using perturbation theory and asymptotic analysis.

We consider the following parametrization, found from a simple perturbation theory sufficiently accurate in the temperature range of experimental interest in the next section:

\[ \xi^{-1}(T) = \xi_0^{-1}(T) \left( \frac{4T}{3T_c} - \frac{1}{3} \right) \]  

\[ \langle \psi^2(T) \rangle = \frac{a'}{b} \left( 1 - \frac{T}{T_c} \right) - \frac{1}{2} k_B = \frac{T_c}{a'} \frac{1}{\sqrt{1 - \frac{T}{T_c}}}, \]  

where \( a' = a(T)/T \). These approximate forms of the parameters \( \langle \psi^2(T) \rangle \) and \( \xi^{-1}(T) \) are used wherever we compare with experiment.

One interesting feature of the exact (numerical) determination of the \( \xi(T) \) is that the correlation length is strictly infinite only at \( T = 0 \) but begins to diverge strongly at a temperature approximately one quarter of the mean field transition temperature. This fact leads to the simple prediction that

\[ T_{3D} \approx T_{MF}/4. \]  

The value of 263 K for \( T_{3D} \) found by experiment (Table 1) is therefore compatible within a fluctuating charge density wave scenario with the estimated \( T_{MF} \) of \( \sim 900K \).

An interesting associated technical question is whether, in a rigorous treatment of the model defined by Equation (1), \( \xi(T) \) actually does diverge at zero temperature, or whether it remains finite due to quantum fluctuations. This depends on properly including the Umklapp processes present in a quarter-filled band. However, for the temperature range \( T > T_{3D} \) which is of interest in this paper quantum fluctuations are not important. For \( T < T_{3D} \), three-dimensional effects dominate in the real system, again suppressing quantum fluctuations.

**Appendix C. Static noncrossing approximation**

Another possible way of calculating the single-particle Green’s function in the static limit is to replace the phonon propagator with delta functions:

\[ D(q, \omega) = \delta_{q \pm 2k_F} \delta(\omega). \]  

and in addition to make the noncrossing approximation that no phonon lines cross. This amounts to calculating the Green’s function self-consistently but neglecting vertex corrections entirely. See Figure 10 for an illustration of this. We shall find that this method leads to unphysical results. It is mentioned only because it is one way of obtaining a pseudogap in a number of different models.
The self energies for two wavevectors are

\[
\Sigma(k, \omega) = \frac{g^2}{\omega - \epsilon_{k-2k_F} - \Sigma(k-2k_F, \omega)} \quad (C40)
\]

\[
\Sigma(k - 2k_F, \omega) = \frac{g^2}{\omega - \epsilon_k - \Sigma(k, \omega)} \quad (C41)
\]

Because of the delta-function effective interaction, these equations close.

Consider first the special case \(k = k_F\). Then \(\Sigma(k, \omega) = \Sigma(k - 2k_F, \omega) = \Sigma(-k_F, \omega)\), \(\epsilon_k = 0\) and

\[
\Sigma(k_F, \omega) = \frac{g^2}{\omega - \Sigma(k_F, \omega)} \quad (C42)
\]

which is a quadratic equation with solution

\[
\Sigma(k_F, \omega) = \frac{1}{2} \omega - \frac{1}{2} \sqrt{\omega^2 - 4g^2} \quad (C43)
\]

The self-energy has a finite imaginary part for \(|\omega| < 2|g|\), i.e., even at zero frequency.

The general case is only slightly more involved. Let us define \(q = k - k_F\) so that \(\epsilon_k = v_F q\) \(\epsilon_{k-2k_F} = -v_F q\). The result is:

\[
\Sigma(q, \omega) = \frac{1}{2} (\omega - \epsilon_k) - \frac{1}{2} \left[ (\omega - v_F q)^2 - 4g^2 \left( \frac{\omega - v_F q}{\omega + v_F q} \right)^2 \right]^{1/2} \quad (C44)
\]

The imaginary part of this function is nonzero when \(|\omega + v_F q| < 2g\).

A finite relaxation time makes no sense for a static, ordered, potential. We conclude that the noncrossing approximation is not appropriate for this problem. This is not surprising. Neglect of vertex corrections is only valid when the electron wavefunctions are only slightly perturbed by the external potential. When degeneracies \((k = k_F)\) or near-degeneracies \((k \approx k_F)\) are a dominant effect, ordinary nondegenerate perturbation theory is not accurate.

**Appendix D. XPS Lineshape and Shift**

We define a core retarded core hole Green’s function

\[
G_h(t) = -i \Theta(t) \langle d^\dagger(t) d \rangle \quad (D45)
\]

and divide it into two parts

\[
G_h(t) = -i \Theta(t) e^{-i\omega_T t} \rho(t) \quad (D46)
\]

where \(\omega_T\) is a threshold energy (containing, in general, contributions from all orders of perturbation theory), and all the relevant many particle effects are consigned to the factor

\[
\rho(t) = \langle |T \exp \left[ -i \int_0^t dt_1 V(t_1) \right] | \rangle \quad (D47)
\]
The lowest order term in a linked cluster expansion for \( \rho(t) \) is
\[
\rho(t) \approx e^{F_2(t)}
\]
\[
F_2(t) = \frac{1}{2} (-i)^2 \int_0^t dt_1 \int_0^t dt_2 \langle TV(t_1) V(t_2) \rangle
\]
\[
= -\frac{1}{2L} \sum_q |V_q|^2 \langle T \rho(q, t_1 - t_2) \rho(-q, t_2 - t_1) \rangle
\]
(D48)

We will confine ourselves here to examining the contribution to the Fermi Edge Singularity (FES) from this term, which contains all the essential physics of the problem.

The expectation value \( \langle T \rho(q, t_1 - t_2) \rho(-q, t_2 - t_1) \rangle \), obviously has the form of a density–density correlation function. We therefore define
\[
i \Pi(q, i\Omega_m) = -\frac{1}{L} \int_0^\beta d\tau e^{i\Omega_m \tau} \langle T \rho(q, t_1 - t_2) \rho(-q, t_2 - t_1) \rangle
\]
(D50)

and introduce a bosonic spectral function \( B(q, \omega) \)
\[
\Pi(q, i\Omega_m) = \int_0^\infty d\tilde{\omega} B(q, \tilde{\omega}) \frac{1 - e^{-i\tilde{\omega}t}}{\tilde{\omega}^2}
\]
(D51)

where \( i\Omega_m \) is a bosonic Matsubara frequency.

Using the general result \( B(q, \tilde{\omega}) = -B(q, -\tilde{\omega}) \), (which follows from analyticity and parity), we find that
\[
\int_0^t dt_1 \int_0^t dt_2 \Pi(q, t_1 - t_2) = 2 \int_0^\infty d\tilde{\omega} B(q, \tilde{\omega}) \frac{1 - e^{-i\tilde{\omega}t}}{\tilde{\omega}^2}
\]
(D52)

and therefore
\[
F_2(t) = -\frac{1}{2L} \sum_q |V_q|^2 \int_0^\infty d\tilde{\omega} B(q, \tilde{\omega}) \frac{1 - e^{-i\tilde{\omega}t}}{\tilde{\omega}^2}
\]
(D53)

where we have dropped terms linear in \( t \) (and therefore belonging in \( \omega_T \)).

In order to be able to apply our analysis to a system with arbitrary spectral function \( A(k, \omega) \) we rewrite the correlation function \( \Pi(q, i\Omega_m) \) in terms of Fermionic propagators, and then substitute a spectral representation of the electrons
\[
G(k, i\omega_n) = \int_0^\infty d\omega' \frac{A(k, \omega')}{i\omega_n - \omega'} = \int_0^\infty d\omega' \frac{A(k, -\omega')}{i\omega_n + \omega'}
\]
(D54)

we find
\[
B(q, \omega) = -2\pi \sum_k \int_{-\infty}^{\infty} d\omega' \frac{A(k + q, \omega' + \omega) A(k, \omega')}{2\pi} \times [n_f(\omega') - n_f(\omega' + \omega)]
\]
(D55)

We Taylor expand
\[
\sum_{kq} \left[ n_f(\epsilon_{k+q}) - n_f(\epsilon_k) \right] \delta(\omega - \epsilon_{k+q} + \epsilon_k)
\]
\[
= -\omega \sum_{kq} \frac{\partial n_f}{\partial \omega} \delta(\omega - \epsilon_{k+q} + \epsilon_k) + \ldots
\]
(D56)
At $T = 0$, $\frac{\partial n_f}{\partial \omega} = -\delta(\omega)$; and we can eliminate both integrals

$$B(q, \omega) = \omega \sum_k A(k + q, \omega) A(k, 0) \tag{D57}$$

We now make the assumption that $V_q$ has no significant $q$ dependence and define the function

$$\tilde{B}(\omega) = \sum_q \frac{B(q, \omega)}{\omega} \tag{D58}$$

In general $\tilde{B}(\omega)$ will also be a function of $l$, where $l$ is an index over scattering channels (in 1D the limiting values $q \approx 0, q \approx 2k_f$). For simplicity we suppress this dependence in what follows.

In terms of $\tilde{B}$ we may write

$$F_2(t) \approx -\frac{1}{L} |V_0|^2 \int_0^\infty d\tilde{\omega} \tilde{B}(\tilde{\omega}) \frac{1 - e^{-i\tilde{\omega}t}}{\tilde{\omega}} \tag{D59}$$

In the physically relevant limit ($\omega \rightarrow 0, t \rightarrow \infty$), and making the substitution $k' = k + q$ we find

$$\tilde{B}(\omega \rightarrow 0) = \sum_{kk'} A(k', \omega \rightarrow 0) A(k, 0) = \left[ \sum_k A(k, 0) \right]^2 = n_0^2 \tag{D60}$$

where $n_0$ is the exact density of states at the Fermi energy.

We impose a soft bandwidth cutoff $\epsilon_0$ (equivalent to having made the substitution $|V_q|^2 \rightarrow |V_0|^2 e^{-q/\epsilon_0} \rightarrow |V_0|^2 e^{-\tilde{\omega}/\epsilon_0}$ in D48), in which case the integral over $\tilde{\omega}$ can be performed exactly to give

$$F_2(t) = -|V_0|^2 n_0^2 \ln(1 + i\epsilon_0 t) \tag{D61}$$

Therefore,

$$G_h(t) \approx -i\Theta(t)e^{-i\omega t} \frac{1}{(i\epsilon_0 t)^{\alpha_E}} \tag{D62}$$

where for a 1D electron system within these approximations and restoring the $2k_f$ scattering channel, the exponent $\alpha_E$ is given by

$$\alpha_E = n_0^2(|V_0|^2 + |V_{2k_f}|^2) \tag{D63}$$

In the special case of free electrons we see that we have recovered the Born Approximation to the exact result.

More generally

$$\alpha_E = \lim_{\omega \rightarrow 0} \frac{1}{L} \sum_q |V_q|^2 \frac{\Re\{\chi(q, \omega)\}}{\omega} \tag{D64}$$

provided that a) the unperturbed Hamiltonian is quadratic in Fermi fields b) the leading small $\omega$ behaviour of $\sum_q |V_q|^2 \Im\{\chi(q, \omega)\}$ is linear.
This form of $G_h(t)$ leads directly to the power law asymmetries in core hole lineshapes observed in experiment. In the case of non-interacting electrons it can be shown that second order perturbation theory represents the Born approximation to the result obtained from resuming all orders of perturbation theory.

\[ \alpha_E = \frac{1}{4} \sum_l \left[ \delta_l(E_f) \right]^2 \]  
\[ (D65) \]

where $\delta_l(E_f)$ is the exact phase shift at the Fermi surface in the $l$'th scattering channel.

It is also possible to calculate the second order shift in the XPS line due to its interaction with the conduction electrons. This may be evaluated as a conventional self energy correction; the result is

\[ \Delta E = \frac{1}{L} \sum_q |V_q|^2 \Re\{\chi_\rho(q,0)\} \]  
\[ (D66) \]

Gross changes in the susceptibility due (for example) to the opening of a gap in a previously ungapped system, can therefore lead to a shift in core lines as well as a change in their asymmetry.

**Appendix E. Core Level coupled to a Luttinger Liquid**

The following model for a localized single Fermion $d$ (chosen here to be a hole) interacting with a set of Bosons $a_q$

\[ H = dd^\dagger \left[ \epsilon_c + \sum_q M_q(a_q + a_q^\dagger) \right] + \sum_q \omega_q a_q^\dagger a_q \]  
\[ (E67) \]

\[ \{d^\dagger, d\} = 1 \left[ a_q, a_{q'}^\dagger \right] = \delta_{qq'} \]  
\[ (E68) \]

may be solved exactly by the canonical transformation

\[ \tilde{H} = e^sHe^{-s} = \tilde{d}d^\dagger [\epsilon_c - \Delta] + \sum_q \omega_q a_q^\dagger \tilde{a}_q \]  
\[ (E69) \]

where

\[ s = dd^\dagger \sum_q \frac{M_q}{\omega_q} (a_q^\dagger - a_q) \quad \Delta = \sum_q \frac{M_q^2}{\omega} \]  
\[ (E70) \]

This model has the unphysical feature that the interaction term does not conserve momentum – the core level does not recoil when electrons are scattered from it.

It is also possible to find the fermion correlation function

\[ iG_d(t) = \langle Td^\dagger(t)d \rangle \]  
\[ (E71) \]

in closed form. We consider only the case $t > 0$, for which the result is

\[ iG_d(t) = [1 - n_f(\epsilon_c - \Delta)] \exp \left[ -\phi(t) \right] \]  
\[ (E72) \]

\[ \phi(t) = \sum_q \left( \frac{M_q}{\omega_q} \right)^2 \left[ N_q \left( 1 - e^{-i\omega_q t} \right) + (N_q + 1) \left( 1 - e^{i\omega_q t} \right) \right] \]  
\[ (E73) \]
where $N_q$ is a boson occupation factor, which we set to zero in what follows. The procedure for solving the model and obtaining correlation functions is described in some detail in [61].

The simplest prototypical Hamiltonian for a core level coupled to interacting conduction electrons in 1D may be written

$$H_1 = \sum_k \epsilon_k c_k^\dagger c_k + \frac{1}{2L} \sum_q V_q \rho(q) \rho(-q)$$  \hspace{1cm} (E74)

$$V_{IMP} = \frac{1}{L} \sum_q M_q \rho(q) d d^\dagger$$  \hspace{1cm} (E75)

$$\rho(q) = \sum_p c_{p+q}^\dagger c_p \hspace{1cm} \{d, d^\dagger\} = 1$$  \hspace{1cm} (E76)

where $\epsilon_p$ is the free electron dispersion and $V_q$ the FT of the electron–electron interaction. This model (the Tomonaga Model) may be solved by linearizing the electron dispersion $\epsilon_p = v_f (|p| - p_f)$ and introducing a set of collective Bosonic coordinates to describe excitations of the conduction electrons.

We now make the observation that the bosonized form of this model is (up to a constant) in exact correspondence with model of a single fermion interacting with a set of bosons solved above.

Explicitly, we split the density operator into separate parts referring to right and left moving electrons $\rho(q) = \rho_1(q) + \rho_2(q)$ which we normalize as bosonic operators

$$b_q = \frac{\pi}{L \pi} [\theta(q) \rho_1(q) + \theta(-q) \rho_2(q)]$$  \hspace{1cm} (E77)

$$[b_q, b^\dagger_{q'}] = \delta_{qq'}$$  \hspace{1cm} (E78)

We write the kinetic energy term as

$$\sum_q \omega_q b^\dagger_q b_q \hspace{1cm} \omega_q = v_f |q|$$  \hspace{1cm} (E79)

and make use of the canonical transformation

$$b_q + b^\dagger_{-q} = \sqrt{\frac{\omega_q}{E_q}} (\alpha_q + \alpha^\dagger_{-q}) \hspace{1cm} [\alpha_q, \alpha^\dagger_{q'}] = \delta_{qq'}$$  \hspace{1cm} (E80)

$$E_q = \sqrt{\omega_q^2 + 4 \omega_q V_q} = v_f |q| \sqrt{1 + \frac{2V_q}{\pi v_f}}$$  \hspace{1cm} (E81)

to obtain

$$H = \sum_q E_q \left(\alpha_q^\dagger \alpha_q + \frac{1}{2}\right) + dd^\dagger \left[\sum_q M_q (\alpha_q + \alpha^\dagger_{-q})\right] + \epsilon_d d d^\dagger$$  \hspace{1cm} (E82)

which is clearly of the same form as (E67).

The density of states at the Fermi energy in a Luttinger Liquid is identically zero and one might expect, on the basis of the arguments presented in Appendix D that this would
mean that it would present no asymmetry in core hole responses. This expectation is not born out — in fact there is no essential difference between the bosonized Hamiltonian for free electrons coupled to a core level and that for interacting electrons coupled to a core level (provided that we neglect all “backscattering” processes). The response of the interacting system is therefore qualitatively the same. However, since the Bosonic eigenstates of the interacting electron system are not exactly the same as those for the free one, we must remember to modify the energy levels and matrix elements in the expression for \( G_d(t) \)

\[
\omega_q \rightarrow E_q
\]

\[
M_q \rightarrow \sqrt{\frac{\omega_q M_q |q|}{2\pi}}
\]

The all important logarithm in the response of the electron system to the impurity may be obtained by replacing the remaining sum over \( q \) with an integral. In the case where all interactions are \( \delta \) functions it is particularly easy to understand what happens.

Then,

\[
\phi(t) = \int_0^{q_0} dq \frac{\overline{M}_q}{2\pi q} \left[ 1 - e^{-iE_q t} \right]
\]

\[
E_q = v|q| \quad \overline{M}_q = \frac{M|q|}{2\pi}
\]

where \( v = v_f \sqrt{1 + 2V/\pi v_f} \) and \( q_0 \) is a band cutoff. We may bring this into the from of the non–interacting case by the change of variables \( \overline{q} = (v_f/\overline{v})q \). Then, without needing to evaluate the integral, we know that the asymmetry exponent will be modified according to

\[
\alpha_E(V) = \left( \frac{v_f}{\overline{v}} \right)^3 \alpha_E(0)
\]

\[
\left( \frac{v_f}{\overline{v}} \right)^3 = \left( 1 + \frac{2V}{\pi v_f} \right)^{-\frac{3}{2}}
\]

i.e. suppression for \( V > 0 \) and enhancement for \( V < 0 \).

A more careful analysis of the \( q \to 0 \) limit of integrand in the general case leads to the result (31) in terms of the Luttinger Liquid correlation parameter of the quoted in the text. The problem of the X–ray response of a LL has been considered previously by a number of authors [32].

It is clear that the approach of Appendix 1 fails dramatically and it is worth pausing to consider why. The result (D53) is quite generally valid at this order. The error arises in the evaluating density–density correlation function \( \Pi(q,i\Omega) \) as a single loop of fermions. In the case of a system with electron–like quasiparticles this is unlikely to lead to a large qualitative error, but in the case of a Luttinger liquid where Wick’s Theorem
does not hold it is quite simply the wrong thing to do. Fortunately it is easy to evaluate the exact form of $\Pi(q, i\Omega)$ by bosonization. Substituting this in (D53) leads to the same results as the approach outlined above.

We note that none of these arguments are affected by the introduction of spin, and may even be applied to an “insulating” phases, if the gap is in the spin rather than the charge sector (Luther–Emery liquid).
Se Rectangles are rotated with regard to one another.

Direction of Ta chain
$\frac{\rho(T)}{\rho(T_{3D})}$ vs. $T \ [K]$
$\rho(T)/\rho(T_{3D})$ vs $T$ [K]

$\sigma(T)/\sigma(T_{3D})$ vs $T/T_{MF}$
\[ \sigma(\omega, T) / \sigma(0.263) \]

Graph showing the relation between \( \sigma(\omega, T) / \sigma(0.263) \) and \( \omega \) in eV, with different curves representing different temperatures: 263 K, 270 K, 300 K, 350 K, 400 K, and 430 K.
\( T \) [K]

\( \eta_0^2 (T) \)

The graph shows the relationship between temperature \( T \) and \( \eta_0^2 (T) \) as a function of temperature.
(a) \[ k_{F+q} = k_{F+q} + k_{F+q} -k_{F+q} k_{F+q} \]

\[ + k_{F+q} -k_{F+q} k_{F+q} -k_{F+q} k_{F+q} \]

\[ + \ldots \]

(b) \[ \Sigma(k_{F+q}) = \]

\[ -k_{F+q} \]

\[ 2 k_F \]

""="" \[ -k_{F+q} \]
