Temperature Dependence of Transport Coefficients in Liquid and Amorphous Metals

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We apply the muffin-tin effective medium approximation to calculate the temperature dependence of the resistivity and of the thermopower of amorphous and liquid metals. The results show unambiguously that a large resistivity is accompanied by a negative temperature coefficient, in agreement with the experimental situation. This behavior is shown to result from a pseudo-gap which opens in the 1-particle spectrum due to strong scattering at the quasi zone boundary. In turn the thermopower is found to have non-trivial density and temperature dependences.

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I. INTRODUCTION

The influence of a disordered potential on the motion of electrons remains an interesting problem despite of decades of work. The aim of solving this problem is to elucidate the properties, if not the existence, of a whole range of materials, such as doped semi-conductors, doped Mott insulators, amorphous and liquid metals, to quote a few. The classes of materials are not only distinguished by the state of their parent compounds, but also by the type of disorder and the influence of the electron-electron interaction. Even if the latter does certainly play a key role for the doped Mott insulators, it is commonly accepted that its role is much reduced in most amorphous and liquid metal systems. Types of disorder can be, among others, “diagonal” as in conventional modeling of doped semi-conductors, doped Mott insulators, amorphous and liquid metals, to quote a few. The classes of materials are not only distinguished by the state of their parent compounds, but also by the type of disorder and the influence of the electron-electron interaction. Even if the latter does certainly play a key role for the doped Mott insulators, it is commonly accepted that its role is much reduced in most amorphous and liquid metal systems. Types of disorder can be, among others, “diagonal” as in conventional modeling of doped semi-conductors, doped Mott insulators, amorphous and liquid metals, to quote a few. The classes of materials are not only distinguished by the state of their parent compounds, but also by the type of disorder and the influence of the electron-electron interaction. Even if the latter does certainly play a key role for the doped Mott insulators, it is commonly accepted that its role is much reduced in most amorphous and liquid metal systems.

The strength of the disorder is an equally important characterization of a physical system. In amorphous, and liquid, metals the disorder is by far not extreme. Instead, neutron scattering data reveal distinct short ranged order (for a review, see [4]), and the ionic structure factor displays a series of peaks. Nevertheless, those metals exhibit a whole range of anomalous properties; especially transport properties exhibit peculiar behavior, and even the electronic structure poses a challenge to the theoretician. How to explain the minimum in the Density of States in noble metal-polyvalent crystalline Hume-Rothery phases [1–4]. Recently Kroha et al. obtained an instability of the Fermi sea towards density oscillations which causes a phase shift of the Friedel oscillations, as well as an enhancement of their amplitude. This instability occurs when the transport time is substantially smaller than the quasi-particle life-time and is consistent with experiment. Experimentally this behavior is best seen when the valence of the glass $Z$ is close to 1.8 el/Atom. In these glasses transport coefficients have been systematically investigated too. As a function of valence, the electrical resistivity is maximum for $Z \sim 1.8$. There it decreases with temperature, while the thermopower grows with the temperature at low temperature. The correlation minimum in the density of states, negative temperature coefficient of the resistivity and positive thermopower has not yet found a definite theoretical explanation.

To tackle this problem we apply the Muffin-Tin Effective Medium Approximation (MT-EMA), to an ensemble of atoms, distributed according to the hard sphere structure factor. Having the electrons moving in the muffin-tin potential created by the atoms is an appealing description of those all-in-all rather good metals. The MT-EMA is a self-consistent scheme which is resumming the disorder averaged multiple scattering series and addresses the 1-particle and 2-particles quantities on an equal footing, so as to fulfill the Ward identities. It precisely allows for a detailed discussion of the interplay of multiple scattering and short ranged order effects. A first study exists [5]. Here we extend it to a complete discussion of the temperature dependence of the electrical resistivity and of the thermopower.
II. SUMMARY OF THE FORMULATION

In this work we investigate the effect of short ranged order (SRO) in an otherwise topologically disordered system, on the electronic structure and transport properties of the medium. Such a question is relevant to metallic glasses and liquid metals, where the periodic arrangement of the ions is replaced by a structure characterized by SRO only. In this case a series of properties of the metals are anomalous. Most striking is the behavior of the electrical conductivity as a function of the temperature. A compilation of experimental data by Mooij leads to the "Mooij rule" and separates the alloys into 2 classes of behaviors: first if the low-temperature resistivity \( \rho_0 \) exceeds a certain threshold value \( \rho_c \) (about 150 \( \mu \Omega \text{cm} \)), then increasing the temperature leads to a decrease of the resistivity, and second if \( \rho_0 < \rho_c \), the more common behavior of seeing the resistivity increasing upon an increase of the temperature is restored. In the meantime, a series of exceptions to the second class of behavior has been discovered, and only the first behavior holds for good. Quite remarkably \( \rho_0 \) is not particularly large, not even 2 orders of magnitude larger than in good metals such as Cu at room temperature. It nevertheless corresponds to a strong reduction of the mean free path down to several atomic spacings. In this regime weak scattering approaches are thus expected to be inappropriate.

Another interesting quantity is the thermopower \( S \). While at low temperature a simple estimate using Boltzmann equation yields \( S/T = -k_\text{B}^2 \pi^2 /|e|E_F \), experimental evidence points towards a very different situation. Not only the magnitude, but even the sign of \( S/T \) are not universal. They strongly depend on the density of charge carriers. The Hall conductivity and the magnetoresistance are anomalous, too, but their investigation is left for future work.

Given the short mean free path, the elucidation of these anomalies is not expected to follow from a simple weak scattering approach, such as Ziman formula for the resistivity. Indeed, as noted by Jäckle, the amplitude of \( S/T \) can be too large to be obtained out of the Ziman formula, even though the general features can be understood in this framework. Moreover the experimental finding of a structure induced minimum in the density of states of noble metal- polyvalent metal glasses by Häussler et al forces us to abandon the nearly free electron model. Instead we resort to the MT-EMA. In this framework free electrons are scattered by the potential of the ions, and the self-energy (which allows for interpreting the results in terms of an effective dispersion relation) is determined by a self-consistent scheme which takes SRO effects into account, by resumming approximately the disorder averaged multiple scattering series. This scheme becomes exact in the limit of large coordination number, provided the Kirkwood superposition principle holds. In real systems the coordination is fairly large (about 11), and allows us to conclude that we have quite a reliable approximation. In turn transport coefficients are determined self-consistently, such as to fulfill Ward identities.

We restrict ourselves to the case of s-scattering only. In sum, we first determine the (disorder averaged) Green’s Function:

\[
< G_k(E) > = G_0(k) + G_0(k)Q_k(k,k)G_0(k) \tag{1}
\]

where the off-shell part of the (disorder averaged) T-matrix is related to the on-shell part at \( \kappa^2 = E \) by:

\[
Q_k(p, p') = n \frac{t(p, p')\tau - t(p, \kappa)t(\kappa, p')}{\tau} + \frac{t(p, \kappa)Q_k(\kappa, \kappa)\tau t(\kappa', \kappa)}{\tau} \tag{2}
\]

the on-shell part of the T-matrix is obtained in terms of its diagonal part \( t_d \) and an effective propagator \( \tilde{G}_k(\kappa) \) as:

\[
Q_k(\kappa, \kappa) = \frac{n t_d(\kappa, \kappa)}{1 - n t_d(\kappa, \kappa)\tilde{G}_k(\kappa)}. \tag{3}
\]

The latter 2 quantities are obtained as the solutions of

\[
\tilde{G}_k(\kappa) = \tilde{B}_k(\kappa) + \int \frac{q^2 dq}{2\pi^2 n} a_0(k, q)\tilde{G}_q(\kappa)Q_q(\kappa, \kappa)\tilde{G}_q(\kappa) t_d(\kappa, \kappa) = t(\kappa, \kappa) + t(\kappa, \kappa) \int \frac{k^2 dk}{2\pi^2} \tilde{G}_k(\kappa)Q_k(\kappa, \kappa)B_k(\kappa) t_d(\kappa, \kappa) \tag{4}
\]

where we have introduced \( t(p, p') \) as the ion off-shell t-matrix, \( B_k(\kappa) \) the effective propagator in the Quasi-Crystalline Approximation

\[
\tilde{B}_k(\kappa) = B_k(\kappa) + \int \frac{q^2 dq}{2\pi^2 n} a_0(k, q)B_q(\kappa) \tag{5}
\]

with \( B_k(\kappa) = 1/(\kappa^2 - k^2) \) being the free electron propagator. The information about the structure enters via the pair distribution function \( h(k) \) (which is related to the structure factor by \( S(k) = 1 + h(k) \)) and the density of the ions \( n \). Expanding the pair distribution function according to:

\[
h(|k - q|) = 4\pi \sum_L Y_L(\hat{k})a_L(k, q)Y_L(\hat{q}) \tag{6}
\]

defines the quantity \( a_0(k, q) \). We obtain the density of states in the usual way:

\[
N(E) = \frac{-2}{n\pi} \int \frac{dk}{(2\pi)^3} \text{Im}(G_k(E)) \tag{7}
\]

and the electronic density by

\[
n_e = \int dE N(E)f(E - \mu). \tag{8}
\]

Next we solve the equations for the transport. The vertex corrections are determined by solving:
\[ X_1(k) = \int \frac{q^2dq}{2\pi^2n} a_1(k,q) \left( \left| \frac{Q_k(\kappa,\kappa)}{nt_d} \right|^2 - 1 \right) X_1(q) \]
\[ + \frac{t(q,\kappa)}{t(\kappa,\kappa)} G_{0q}(E)Q_q(\kappa,\kappa)^2 q \]
\[ X_2(k,k') = \int \frac{q^2dq}{2\pi^2n} a_1(k,q) \left( \frac{G_{0q}(E)Q_q(\kappa,\kappa)X_2(q,k')}{nT_d} \right) \]
\[ + \frac{t(q,\kappa)}{t(\kappa,\kappa)} G_{0q}(E)Q_q(\kappa,\kappa)^2 q G_{0q}(E') \]
\[ \left( \frac{t'(q,k')t' - t'(q,\kappa)t'(\kappa,k)}{t'(\kappa,\kappa)} \right) \]
\[ X_3(k) = \int \frac{q^2dq}{2\pi^2n} a_1(k,q) \]
\[ \left| \frac{t(q,\kappa)t(\kappa,\kappa) - t(q,\kappa)t(\kappa,k)}{t(\kappa,\kappa)} G_{0q}(E) \right|^2 q \]
out of which we construct:
\[ \Lambda_k(E) = \left| \frac{t(k,\kappa)}{t(\kappa,\kappa)} Q_k \right|^2 X_1(k) \]
\[ + 2Re \left( \frac{t(k,\kappa)}{t(\kappa,\kappa)} Q_k X_2(k,k) \right) + X_3(k) \]
which allows for obtaining the \( E \)-dependent conductivity
\[ \sigma(E) = \frac{h^2}{3\pi m} \int \frac{k^3dk}{2\pi^2} \left( G_{0k}(E^+)G_{0k}(E^-) \Lambda_k(E) \right) \]
\[ - \frac{m}{h^2} Re \left( G_k^2(\kappa^+)\frac{d\Sigma_k(\kappa^+)}{dk} \right) \]
\[ + \frac{h}{3\pi m} \int\int dk k^4 \left( \frac{\text{Im}(G_k(E))}{\pi} \right)^2 \]
out of which the conductivity results into:
\[ \sigma = \int_{-\infty}^{\infty} dE \frac{-\partial f_E}{\partial E} \sigma(E) \]

We shall compare the EMA conductivities to the ones following from Ziman formula
\[ \rho_{Ziman} = \frac{3\pi n}{4\hbar^2 v_f^2 k_F^4} \int_0^{2k_F} dq q \int S(q) |t(\kappa,\kappa)(E_F)|^2 . \]
\[ \text{(13)} \]

In linear response the thermopower \( S \) results into:
\[ S = -\frac{1}{eT} \int_{-\infty}^{\infty} dE \frac{\partial f_E}{\partial E} (E - \mu) \sigma(E) \]
\[ \text{(14)} \]
For more details we refer to \[32\].

### III. RESULTS

We first describe how the atomic structure is taken into account. Here we resort to the Percus-Yevick solution of the hard sphere liquid to model the ionic structure. The resulting structure factor is displayed in fig. 1, for packing fractions \( \eta \) ranging from \( \eta = .38 \) to \( \eta = .42 \), which are reasonable values in order to account for at least liquid simple metals.

Even though merely a model structure factor, it is expected to capture the main features of the structure, and has been favorably compared to the one of liquid simple metal. It also has the advantage of substantially reducing the numerical effort since \( h(k) \) has an analytical expression. Here the height of the first peak of the structure factor can be varied by tuning the packing fraction, in order to mimic a change in temperature. In order to model the dependence of \( \eta \) on \( T \), we have reported the height of the first peak of the structure factor \( S(k_F) \) as a function of temperature for various systems in fig. 1.

Applying a best fit procedure reveals that \( S_T(k_F) \) obeys a law:
\[ S_T(k_F) = \frac{1}{aT + b} \]

sticking to liquid Rb for the sake of definiteness yields \( a = 5.09 \times 10^{-4} K^{-1} \) and \( b = 0.23378 \). We can then model the temperature dependence of \( \eta(T) \), listed in table 1.

| TABLE I. Temperature dependence of the packing fraction |
|--------------------------|----------|----------|----------|----------|
| \( T[K] \)     | 430      | 463      | 499      | 537      | 573      |
| \( \eta \)     | .32      | .41      | .40      | .39      | .38      |

| \( S(k_F) \) | 2.08 | 2.129 | 2.049 | 1.970 | 1.901 |

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[32] Reference to be included.
We use the square well potential to model the screened Coulomb potential of the ions. In atomic units it is described by the parameter \( V_z = V a^2 \), where \( V \) is the depth of the potential and \( 2a \) its range. Throughout this work we use \( V_z = 1.4 \) and the unit \( \hbar = 2m = e^2 = 1 \).

\[ \text{FIG. 2.} \quad \text{The amplitude of the first peak of the structure factor } S(k_p) \text{ as function of temperature.} \quad [29] \quad 1: \text{liq. Al (6), 2: liq. CuSn (1), 3: liq. GeTe (2), 4: liq. AlGe (3), 5: liq. Ga (4), 6: liq. Sn (4), 7: liq. Cd (4), 8: liq. Zn (4), 9: liq. Zn (5), 10: liq. Rb (7), 11: liq. Cs (8), 12: liq. Ga (9), 13: liq. Rb (10), 14: amor. MgZn (11), 15: amor. CaZn (11), 16: amor. MgCu (11), 17: liq. Zn (12), 18: liq. Rb [23].} \]

**A. Electronic structure**

We now proceed to solve the set of equations (4), determining the electronic structure. To some extent these equations have been solved by Frésard et al. Here we solve them in order to first determine the parameter range where the theory is analytic. Indeed the breakdown of analyticity of the MT-EMA has been observed for the delta-function potential by Singh and Roth possibly yielding negative spectral functions especially for large packing fractions, and no proof of analyticity of the approximation has been found. It turns out that the analyticity breaks down for low Fermi energies, when \( \eta > 0.44 \), namely a value which is above those we are dealing with in this work. For \( \eta \le 0.42 \), the theory is analytic for all values of the potential and of the Fermi energy. The main result concerns the density of states and is displayed in fig. 3. Two features appear clearly. First a deep minimum, and second quite a sizeable peak just below it. The minimum is becoming deeper and deeper as \( \eta \) is growing and occurs at \( E_m \), with \( E_m \sim (k_p/2)^2 \) with little dependence on the potential strength. It is thus fair to say that it results from quasi Bragg scattering on a quasi zone boundary. It replaces the energy gap which opens when the lattice periodicity is restored. As a result breaking the periodicity of the lattice does not invalidate the concept of zone boundary as a whole: even though the latter cannot be defined as the inverse of the lattice spacing but is rather given in an effective way by about \( k_p/2 \), it still locates the region in k-space where a pseudo-gap opens due to strong backscattering. At \( E_m \), and below it, the effective dispersion flattens which leads to the maximum in the density of states. Such a maximum leads to a decrease in the total energy making it very likely to find most real liquid and amorphous metals with a Fermi energy close to \( E_m \), in agreement with the argument of Nagel and Tauc.

\[ \text{FIG. 3.} \quad \text{The electronic density of states, for the potential strength } V_z = 1.4 \text{ and for different packing fractions. The dashed curve corresponds to the calculated free electron density of states. Inset: expanded view around } E_m. \]

\[ \text{FIG. 4.} \quad \text{The density of electrons, for the potential strength } V_z = 1.4 \text{ and for different packing fractions. Inset: expanded view around } E_m. \]
The dependence of the charge carrier density on the Fermi energy is displayed in fig. 4, and it appears that \( E_m \) corresponds to \( n_m = 1.78 \). This value is not universal, and depends on both \( V_z \) (clearly) and \( \eta \) (weakly). Typically it will be shifted down to lower densities by reducing \( V_z \), or increasing \( \eta \). Note that the lower band edge is shifted down from 0 due to the averaged attractive potential. More details concerning the spectral function, the self-energy and the effective dispersion can be found in \( 15, 22 \).

**B. Electrical Resistivity**

We now proceed to the solution of the transport equations Eq. (9). The result is displayed in fig. 5, where we display the conductivity as a function of the electronic density for several temperatures.

![Diagram showing conductivity as a function of temperature and density](image)

**FIG. 5.** The electrical conductivity, for the potential strength \( V_z = 1.4 \) at different temperatures, calculated in EMA and with the Ziman formula.

For each temperature the conductivity has a deep minimum at \( n_e \sim 1.8 \), corresponding to \( E_m \) (see above). This minimum does not only follow from the short life time of the quasi-particles, but from large vertex corrections too. It becomes deeper and deeper as the temperature is lowered. Note that the bundle of curves crosses at \( n_e \sim 1.5 \) and \( n_e \sim 2.5 \), namely where the bundle of density of states crosses too.

This is the root of the Mooij rule. Due to strong multiple scattering at the pseudo zone boundary, a pseudo-gap opens in the 1-particle spectrum, which becomes deeper and deeper as SRO grows. In turn it induces a minimum in the conductivity which itself is getting deeper and deeper as SRO grows, namely as the temperature decreases. It thus turns out that the resistivity decreases as the temperature increases, when the resistivity is small.

In more detail the temperature dependence of the resistivity is displayed in fig. 6 for several values of the electronic density. In the regime of low electronic density \( (n_e \leq 1.7) \) where \( E_F < E_m \), the resistivity increases with temperature at a moderate rate. When the electronic density \( n_e \) approaches \( n_m \) than the resistivity \( \rho \) decreases with increasing temperature \( T \) at a higher rate. It is maximum at \( n_m \). A further increase in the density leads to a decrease of this rate, for \( n_e \) up to 2.4 where it changes its sign.

![Diagram showing resistivity as a function of temperature and density](image)

**FIG. 6.** The resistivity as function of temperature, for the potential strength \( V_z = 1.4 \) and for different densities of electrons.

Those data can be summarized by reporting the temperature coefficient of the resistivity \( \alpha \):

\[
\alpha \equiv \frac{1}{\rho} \frac{\partial \rho}{\partial T} \quad (16)
\]

as a function of the resistivity. Calculating \( \alpha \) at the lowest temperature leads to fig. 7.
The data scatter onto 2 lines which represent the 2 regimes where the Fermi energy is either smaller or larger than $E_m$. Not only the sign of $\alpha$, but its magnitude as well, compare favorably with the experimental results. In contrast to ref. 15, we have calculated the temperature dependence of the resistivity for fixed density. There are 3 contributions to $\alpha$: (i) the $\eta$-dependence of the resistivity as such, (ii) the smearing of the Fermi surface together with a strong $E$-dependence of $\sigma(E)$, (iii) the change in the Fermi energy (at fixed density) following from a change in $\eta$ and $T$.

The first contribution to $\alpha$ is dominated by 1-particle effects and has been discussed above. This is the leading one. The second one results from the curvature of $\sigma(E)$ as one can infer it from the Sommerfeld expansion, and is contributing to $\alpha$ in much the same way as the first one; namely the curvature of $\sigma(E)$ is positive in the vicinity of $E_m$, negative below it, and very small above it. This is the second leading one. The third contribution, however, works in the opposite direction, and reduces the value of $\alpha$ at $E_m$.

C. Thermopower

We now evaluate the thermopower according to Eq. (14) and we display it in fig. 8 where it is compared to the results obtained out of the Ziman formula.

As compared to the results obtained out of the Ziman formula, we obtain much larger values, either positive if $E_F < E_m$ or negative if $E_F > E_m$. Again the position of the Fermi energy with respect to $E_m$ plays the key role for assessing the sign of the thermopower. It changes its sign when the resistivity reaches its maximum value.

Thus phononic mechanisms are not required to explain the experimentally observed large values of $S$, even though they are certainly going to play an important role as well, especially around the Debye temperature. Another important contribution, namely the phonon drag effect, is however small in metallic glasses because the scattering of the phonons by the high degree of disorder keeps them essentially in local thermal equilibrium.

We turn to the $T$-dependence of $S$ and display it on fig. 9.

Typically it is growing with the temperature when the Fermi energy is smaller than $E_m$, whereas it is decreasing when $E_F > E_m$. If $E_F$ is within $k_B T$ of $E_m$, there is a crossover region where $\partial S/\partial T$ can have ei-
ther sign. Namely, if $E_F < E_m$, we have $\partial S/\partial T > 0$ if $k_BT < E_F - E_m$ and $\partial S/\partial T < 0$ if $k_BT > E_F - E_m$. On the other hand, if $E_F < E_m$, we have $\partial S/\partial T < 0$ if $k_BT < E_F - E_m$ and $\partial S/\partial T > 0$ if $k_BT > E_F - E_m$. Such a behavior has been observed in noble metals- polyvalent metals alloys such as (Au, Ag, Cu) - Sn. Indeed increasing the content of Sn (i.e. the density of charge carriers) changes the sign of the thermopower at low temperature from positive to negative while the resistivity decreases as review by Häussermann. We finally note that the values of $S$ are too large to fit the experiments from the relatively sharp E-dependence of the density of states, which is strongly reflected in the thermopower. The situation should improve by including multiple occupancy corrections to the theory, but this is beyond the scope of this work.

IV. SUMMARY AND ACKNOWLEDGMENT

In summary we have solved the MT-EMA equations for a system of s-scatterers. The results lead us to a consistent interpretation of the anomalous transport properties of amorphous metals. Especially we found that if the resistivity exceeds a certain threshold, than it decreases with increasing temperature, while otherwise the temperature coefficient of the resistivity can have either signs. This behavior follows from the opening of a pseudo-gap at the quasi zone boundary. The pseudo-gap is responsible for a large resistivity, as well as for a large thermopower (which can be positive or negative) and its non-trivial temperature dependence. As a function of the charge carrier density, the low temperature thermopower changes its sign when the resistivity reaches its maximum.

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V. APPENDIX

In order to solve the set of equations Eq.(1) numerically we use a set of transformations in order to make the task tractable. First we solve the equations for complex energies with $\text{Im}(E) = 1$ which turns out to be easy to solve. We then gradually reduce $\text{Im}(E)$ down to $10^{-4}$, a value that is typically smaller than $-\text{Im}(\Sigma(k_F))$ which has thus very little influence on the result. The equations will be solved by iteration. Even though we use a linear combination of the previous 3 iterations to improve the convergence, the combination being chosen so as to optimize the difference between the input and the output, the task turn out to be very tedious and require as much as $10^3$ iterations for each value of $\eta$ and $E_F$. We handle the on-shell singularity which enters the expression for $G_k(k)$ in the same way as described in ref.(15) namely we introduce:

$$\hat{G}_k(k) \equiv G_k(k) - B_k(k)$$

$$\Sigma_d \equiv \frac{1}{t(k, \kappa)} - \frac{1}{t_d(k, \kappa)}$$

which obeys the equations:

$$\hat{G}_k(k) = \int \frac{q^2 dq}{2\pi^2} a_0(k, q)$$

$$1 - t(k, \kappa)B^{-1}_q(k)\hat{G}_q(k)^2 + nt(k, \kappa)\hat{G}_q(k)$$

$$B^{-1}_q(k)(1 - t(k, \kappa)(\Sigma_d + n\hat{G}_q(k))) - nt(k, \kappa)$$

$$\Sigma_d = nt(k, \kappa) \int \frac{k^2 dk}{2\pi^2}$$

$$\frac{B_k(k) + \hat{G}_k(k)}{B^{-1}_q(k)(1 - t(k, \kappa)(\Sigma_d + n\hat{G}_q(k))) - nt(k, \kappa)}$$

Nevertheless, even though the new equation is now smooth on-shell, it will develop a singular behavior at the renormalized quasi-particle peak through the T-matrix. The difference is that the location of the pole is not known beforehand, and lies in the complex plane. Thus some additional manipulations of the equations is required. They are inspired by considering the integral:

$$\int \frac{f(x)}{x - z} dx$$

The integrand is singular at $z, z$ being complex. If $\text{Im}(z)$ is large, the resulting integrand is smooth and such an integral can be evaluated as such. But when $\text{Im}(z)$ is small, it is best to transform the integral Eq.(19)

$$\int \frac{f(x)}{x - z} dx = \int \frac{f(x) - f(z)}{x - z} dx + f(z) \int \frac{1}{x - z} dx$$

and evaluate the second term analytically. Obviously the resulting integrand is smooth. Applying this principle to Eq.(19) allowed us to greatly improve the numerical stability of the scheme.

Another difficulty arises because the integrands in Eq.(19) decrease slowly for large momenta. In this case we have:

$$1 - t(k, \kappa)\Sigma_d + nt(k, \kappa)B^{-1}_q(k)\hat{G}_q(k)^2 + nt(k, \kappa)\hat{G}_q(k)$$

$$B^{-1}_q(k)(1 - t(k, \kappa)(\Sigma_d + n\hat{G}_q(k))) - nt(k, \kappa)$$

$$\frac{q^2 dq}{2\pi^2} a_0(k, q) \begin{cases} \equiv \frac{1}{2\pi^2 n} a_0(k, q) \end{cases}$$

Defining

$$H(k) \equiv \int_{k_{cut}}^{\infty} \frac{-dq}{2\pi^2 n} a \frac{a_0(k, q)}{q^2}$$

(22)
we also obtain the large momenta contribution to Σ_d as
\[
\theta_d \equiv \frac{-nt(\kappa, \kappa)}{l(\kappa, \kappa)\Sigma_d} \int_{k_{\text{cutoff}}}^{\infty} \frac{dk}{2\pi^2} (B_\kappa(k) + H(k))
\]
which is added to Σ_d at each iteration, in the same way as H(k) is added to \( \tilde{G}_\kappa(k) \). Both integrals entering Eq. \ref{eq:23} can be calculated once and for all.

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