

Single Particle Green's Functions Calculation of the Electrical Conductivity of Strong Correlated Systems

WALDIR A. RODRIGUES, JR.*§

Massachusetts Institute of Technology, Cambridge, Ma 02139, USA

Recebido em 13 de Março de 1978

A calculating of the electrical conductivity for Hubbard materials is presented which is valid when $U/t \gg 1$ (U being the Coulomb repulsion and t the nearest neighbor hopping energy) for arbitrary electron concentration and temperature. The derivation employ the single particle real and imaginary times Green's functions instead of the usual two-particle real time Green's function. The result is compared with the experimental data available for some organic charge transfer salts.

Apresentamos um cálculo da condutividade elétrica para "materiais de Hubbard" válido quando $U/t \gg 1$ (U sendo a repulsão Coulombiana, t a energia de transferência para vizinhos próximos) para concentração eletrônica e temperatura arbitrárias. A dedução emprega as funções de Green com tempos real e imaginário, em vez do método usual que emprega a função de Green de duas partículas. O resultado é comparado com dados experimentais disponíveis para alguns sais orgânicos com transferência de carga.

1. INTRODUCTION

There are some materials characterized by *narrow energy bands* where strong electron correlation plays the major role. The importance of these correlations in narrow energy bands was dramatically illustrat-

* On leave from Instituto de Física-UNICAMP, 13100 Campinas, Brazil.

§ Supported in part by FAPESP, São Paulo, Brazil, Contract 76/0549.

ed by Adler¹ in his analysis of the electronic structure of transition metal oxides. For example, MnO is predicted to be metallic according to band theory and it is experimentally an insulator.

A model for electronic correlations has been developed by Hubbard². There, an electron in a narrow energy band is supposed to hop from site to site in the lattice with a hopping frequency of the order of the bandwidth. When it happens to come onto an atomic site already occupied by an electron of opposite spin it experiences a strong repulsion force. U being the intra-atomic Coulomb energy, a narrow band is then defined as one in which U is large compared with the bandwidth. Hubbard showed² using Green's functions techniques that the excitation spectra of the correlated electron system (in the non-magnetic case) corresponds to the splitting of each of the original bands into two sub-bands. It is important to emphasize here that these new bands are in fact many particle excitation spectra of a nature different from the original bands which as is well known are a consequence of the solution of an electron Schrödinger equation in a periodic lattice. We will turn to this point again.

The Hubbard Hamiltonian has been a subject of intense research.³ Very interesting results exist for the model in one dimension. The excitation spectra has been studied by several authors^{4,5,6,7} and the results applied to the study of the magnetic susceptibility, spin waves, etc. in organic metals like TTF-TCNQ to mention an example.^{8,9}

Using a *one electron picture*, where the one electron states are taken to be occupation number dependent in a simpler manner Yoffa and Adler^{10,11} derived the Fermi energy, specific heat and thermal conductivity of the so-called Mott insulators. Also, the electronic conductivity and thermopower has been studied within this one electron picture.^{12,13,14}

More general results for the electric conductivity and inter-band transitions has been obtained by Kubo¹⁵ using a decoupling scheme for the two particle, real time, temperature dependent Green's functions.

The use of perturbation methods using imaginary time Green's functions and the associated Feynman graphs are difficult to apply to the Hubbard Hamiltonian with strong intrasite repulsion due to the lack of a suitable perturbation parameter. When the concentration is small, however,

we can use something like the ladder approximation of the imperfect Fermi gas. Lyo¹⁶ studied the transport properties in this case and found for the conductivity results which are identical to the one obtained by Kubo.

In the present paper we use the single particle real and imaginary time, temperature dependent Green's functions formalism to calculate the electrical conductivity up to order t^2 (t , being the nearest-neighbor hopping energy-supposed small relative to U) at arbitrary concentration and temperature.

As a first step in the calculation we derive in sections 2 and 3, with the aid of the Green's functions formalism, the Fermi energy and the internal energy in the atomic limit of the Hubbard model. We also discuss briefly the question of the band splitting which has been a source of some misconception.

In section 4 the results obtained are inserted in the Kubo formula and in this way the conductivity is easily obtained. Finally, in section 5 we show that the formula we get predicts under the relaxation time approximation (with a single temperature dependence for τ_e) the conductivity of NMP-TCNQ, but is at variance with the data for TTF-TCNQ.

2. REAL TIME GREEN'S FUNCTION AND THE CHEMICAL POTENTIAL

We consider in the following a system of N interacting electrons described by the Hubbard Hamiltonian

$$H = \sum_{i,j=1}^N \sum_{\sigma} t_{ij} c_{i\sigma}^{\dagger} c_{j\sigma} + U \sum_{i=1}^N n_{i\uparrow} n_{i\downarrow} \quad (1)$$

$n_{i\sigma} = c_{i\sigma}^{\dagger} c_{i\sigma}$ is the occupation number of site i ($i = 1, 2, \dots, N$) and $c_{i\sigma}^{\dagger}$ and $c_{i\sigma}$ are respectively the creation and annihilation operators of an electron with σ spin at the i th atomic site, t_{ij} is the transfer matrix element between the i th and j th site. U is the repulsive potential which acts only when two electrons with opposite spin are at the same site. The band energy is related to t_{ij} through

$$\epsilon_{k\sigma} = \sum_{ij} t_{ij} e^{i\vec{k} \cdot (\vec{R}_i - \vec{R}_j)} \quad (2)$$

In the atomic limit, where $t_{ij} = 6_{ij} T_0$, the Fourier transform of the causal, retarded and advanced, real time, temperature dependent Green's functions (see appendix for the definitions) which give the spectra of pseudo-particles of the system, can be obtained exactly using the equation of motion method described by Zubarev.¹⁷ We obtain for the analytic continuation of both the advanced and the retarded Green's function in the complex energy plane, the equation

$$\Gamma_{ij}^{\sigma\sigma'}(E) = \delta_{\sigma\sigma'} \delta_{ij} \left[\frac{1 - \langle n_{i\sigma} \rangle}{E + \mu - T_0} + \frac{\langle n_{i\sigma} \rangle}{E + \mu - T_0 - U} \right] \quad (3)$$

μ is the chemical potential which fixes the number of particles and $\langle n_{i\sigma} \rangle$ is the thermal average of the expectation of $n_{i\sigma}$ over a grand canonical ensemble at temperature T . In what follows we assume $\langle n_{i\sigma} \rangle = n_\sigma = \frac{1}{2} n$, where n is the number of electrons per atom. This restricts our discussion to nonmagnetic states. The mean number of electrons per atom can be obtained through the expression:

$$\begin{aligned} n &= N^{-1} \sum_{j\sigma} \langle c_{j\sigma}^\dagger c_{j\sigma} \rangle \\ &= \frac{i}{N} \lim_{\eta \rightarrow 0^+} \sum_j \text{tr} [\Gamma_{jj}(\omega + i\eta) - \Gamma_{jj}(\omega - i\eta)] \frac{d\omega}{e^{\beta\omega} + 1} \\ &= \frac{2i}{N} \lim_{\eta \rightarrow 0^+} \sum_j \int [\Gamma_{jj}(\omega - \mu + i\eta) - \Gamma_{jj}(\omega - \mu - i\eta)] \frac{d\omega}{e^{\beta(\omega-\mu)} + 1} \end{aligned} \quad (4)$$

In Eq.(4) as usual $\beta = 1/kT$. From this equation we immediately infer that the pseudoparticles density of states per atom is given by

$$\begin{aligned} \rho(E) &= \frac{2i}{N} \lim_{\eta \rightarrow 0^+} \sum_j [\Gamma_{jj}(E - \mu + i\eta) - \Gamma_{jj}(E - \mu - i\eta)] \\ &= (2-n) \delta(E - T_0) + n\delta(E - T_0 - U) \end{aligned} \quad (5)$$

The Fermi energy $\epsilon_F(n, T) \equiv \mu$ can be immediately calculated from Eq. (4) by solving the equation

$$n = \int dE \rho(E) \frac{1}{e^{\beta(E-\mu)} + 1} \quad (6)$$

We find:

$$\mu = T_0 - kT \ln \left[\frac{(1-n) + \sqrt{(1-n)^2 - n(n-2)} e^{-\beta U}}{n} \right] \quad (7)$$

With some algebraic manipulations Eq. (7) can be put in the alternative form

$$\mu = T_0 + U + kT \ln \left[\frac{(1-n) - \sqrt{(1-n)^2 - n(n-2)} e^{-\beta U}}{(n-2)} \right] \quad (8)$$

which is the result obtained by Yoffa and Adler¹⁰.

3. THE INTERNAL ENERGY

In order to obtain the internal energy we need to know the Fourier transform of the imaginary time Green's function. This can be obtained as follows¹⁸. We first transform $\Gamma_{ij}(E)$ from the Wannier to the basis introducing $\Gamma(\vec{k}, E)$ through

$$\Gamma_{ij}(E) = N^{-1} \sum_{\vec{k}} \Gamma(\vec{k}, E) \exp[ik \cdot (\vec{R}_i - \vec{R}_j)] \quad (9)$$

Then,

$$\Gamma(\vec{k}, E) = \frac{1}{N} \left[\frac{1 - \frac{1}{2}n}{E + \mu - T_0} + \frac{n/2}{E + \mu - T_0 - U} \right] \quad (10)$$

Next introducing the operator function $\rho(\vec{k}, \omega)$ defined through

$$\rho(\vec{k}, \omega) = 2\Gamma(\vec{k}, \omega - i\eta) \quad (11)$$

we obtain $G(\vec{k}, \omega_\ell)$, where $\omega_\ell = (2\ell + 1)\pi\beta$ is the fermion frequency through the equation

$$\begin{aligned} G(\vec{k}, \omega_\ell) &= \int_{-\infty}^{\infty} \frac{d\omega'}{2\pi} \frac{\rho(\vec{k}, \omega')}{i\omega_\ell - \omega'} \\ &= \frac{1}{N} \left[\frac{1 - n/2}{i\omega_\ell + \mu - T_0} + \frac{n/2}{i\omega_\ell + \mu - T_0 - U} \right] \end{aligned} \quad (12)$$

The energy per atom is then

$$\begin{aligned} \frac{E}{N} &= \frac{1}{\beta} \lim_{\eta \rightarrow 0^+} \sum_{\vec{k}} \sum_{\ell} e^{i\omega_\ell \eta} \frac{1}{2} (i\omega_\ell + \epsilon_{k\sigma} + \mu) \text{tr} G(\vec{k}, \omega_\ell) \\ &= 2 T_0 \left(1 - \frac{n}{2}\right) \frac{1}{e^{\beta(T_0 - \mu)} + 1} + (2T_0 + U) \frac{n/2}{e^{\beta(T_0 + U - \mu)} + 1} \end{aligned} \quad (13)$$

Eq. (13) can be put in a compact form using the value of μ given by Eq. (8).

$$\frac{E}{N} = nT_0 + \frac{nU}{2[1 + e^{\beta(T_0 + U - \mu)}]} \quad (14)$$

which agrees with the value obtained in Ref.9, using an appropriate grand partition function for N independent atomic sites.

For the calculation of the conductivity we shall need the value of the thermal average $\langle n_{i\uparrow} n_{i\downarrow} \rangle$. It is obvious from the form of the Hubbard Hamiltonian that this number is given by $N^{-1}U^{-1} \langle V \rangle$, where $\langle V \rangle$ is the thermal average of the interaction energy. We then have

$$\begin{aligned} \langle n_{i\uparrow} n_{i\downarrow} \rangle &= \frac{1}{NU} \langle V \rangle = \frac{1}{U} \frac{1}{\beta} \lim_{\eta \rightarrow 0^+} \sum_{\vec{k}} \sum_{\ell} e^{i\omega_\ell \eta} \frac{1}{2} (i\omega_\ell - \epsilon_{k\sigma} + \mu) \text{tr} G(\vec{k}, \omega_\ell) \\ &= \frac{n}{2[1 + e^{\beta(T_0 + U - \mu)}]} \end{aligned} \quad (15)$$

In Ref. 9 the above results have been obtained through the introduction of a grand partition function Z for N independent sites which can be completely unoccupied ($E = 0$ nondegenerate), single occupied ($E = T_0$ twofold degenerate) or doubly occupied ($E = 2T_0 + U$, nondegenerate).

Using the single electron picture it seems that the states of the upper band appear as consequence of sites which are doubly occupied. Then it seems natural to answer the question — how many electrons per atom are there in the upper band at a given temperature? — simply by saying that these are the number of doubly occupied sites. This number $n_u^s(T)$ is according to the single electron picture

$$n_u^s(T) = \frac{n}{2 \left[1 + e^{\beta(T_0 + U - \mu)} \right]} \quad (16)$$

According to the Green's function formalism the same question is answered through Eq. (6) and we get

$$n_u^g(T) = \frac{n}{1 + e^{\beta(T_0 + U - \mu)}} \quad (17)$$

As this result doesn't agree with Eq. (16) [although we remind that both methods give the same results for the Fermi and internal energies] we must find an explanation for the situation.

What happens is that the Green's functions formalism (as opposed to the single particle picture under which the grand partition function of Ref. 10 was constructed) implies that the upper band exists once and for all when the interaction between electrons is switched on. So there is a nonzero probability for an electron which is in a single occupied site to be excited in the upper band (when $T \neq 0$). This is why we got different results from the two methods. We may infer from the above discussion that the question about which point of view is the correct one can be answered from a calculation of the conductivity, since at first sight this quantity seems to depend on the relative population of the bands. As we shall see in section 4 the calculation of the conductivity (to order t^2) reduces to the knowledge of the thermal average of doubly

occupied sites and for this reason both methods give the same answer again. To end this section we would like to emphasize that the subbands are *many particle pseudo-particle excitation spectra* which arise due to the electron correlation and are there as a whole once and for ever. Obviously the shapes of the subbands depend on the particular material, being determined by U , t and n .

4. CALCULATION OF THE CONDUCTIVITY

We now use the results of sections 2 and 3 to calculate the conductivity to order $t^2 (U/t \gg 1)$. We suppose that the t_{ij} 's in Eq. (1) are different from zero and equal to t for nearest neighbors only. The dissipative part of the electric conductivity tensor is given by Kubo¹⁹ formula

$$\sigma_{\mu\nu}(\omega) = \frac{i}{V} \lim_{\eta \rightarrow 0^+} \int_0^\infty \langle [j_\mu^i(t), \chi_\nu] \rangle e^{-i\omega t - \eta t} dt \quad (18)$$

where V is the volume of the system, j_μ^i is the μ component of the current operator and χ_ν is the ν component of the electric polarization operator. In Wannier basis we have,

$$\vec{\chi} = e \sum_{i\sigma} \vec{R}_i n_{i\sigma} \quad (19)$$

$$j_\mu = \frac{d}{dt} \chi_\mu - i e \sum_{ij\sigma} t_{ij} (\vec{R}_i - \vec{R}_j)_\mu c_{i\sigma}^\dagger c_{j\sigma} \quad (20)$$

and $j_\mu(t) = e^{iHt} j_\mu e^{-iHt}$ is the Heisenberg representation of j_μ . Eq. (18) can be written in the alternative form

$$\sigma_{\mu\nu}(\omega) = \frac{1}{2V} \int_{-\infty}^\infty d\tau e^{i\omega\tau} \int_0^\beta \langle j_\mu(0) j_\nu(\tau + i\lambda) \rangle d\lambda \quad (21)$$

It what follows we assume σ diagonal. In this case \vec{R}_i are the components of the lattice-site position vectors parallel to the external field.

Using Eq. (20) we obtain

$$\sigma(\omega) = \frac{e^2}{2V^2} \sum_{\substack{i,j\sigma \\ k,l\sigma'}} (R_i - R_j) (R_k - R_l) t_{ij} t_{kl} \\ \times \int_{-\infty}^{\infty} d\tau e^{i\omega\tau} \int_0^{\beta} d\lambda \langle c_{i\sigma}^+ c_{j\sigma} e^{iH(\tau+i\lambda)} c_{k\sigma}^+ c_{l\sigma} e^{-iH(\tau+i\lambda)} \rangle \quad (22)$$

In general the calculation of

$$\langle c_{i\sigma}^+ c_{j\sigma} e^{iH(\tau+i\lambda)} c_{k\sigma}^+ c_{l\sigma} e^{-iH(\tau+i\lambda)} \rangle \quad (23)$$

requires knowledge of the two-particle real time, temperature dependent Green's function, but if we are interested in an approximation for the conductivity to order t^2 , then the single particle imaginary time Green's function is enough. This is due to the fact that all contributions of order greater (and equal to) than t^2 to the conductivity comes from the calculation of Eq. (23). This means that to obtain the contribution of order t^2 we must calculate Eq. (23) in zero order in t . This can be done by the substitution

$$H \rightarrow U \sum_i n_i^\uparrow n_i^\downarrow \quad (24)$$

Then

$$\sigma(\omega) = e^2 a^2 t^2 g \eta \int_{-\infty}^{\infty} d\tau e^{i\omega\tau} \int_0^{\beta} d\lambda \langle e^{iU(\tau+i\lambda)(n_{k-\sigma} - n_{l-\sigma})} n_{l\sigma} (1 - n_{k\sigma}) \rangle \quad (25)$$

where a is the lattice spacing, g is the number of nearest neighbors and η is the number density ($\eta = N/V$). The thermal average in Eq. (25) decouples in our approximation in

$$\langle e^{iU(\tau+i\lambda)n_{k-\sigma}} (1 - n_{k\sigma}) \rangle \langle e^{-iU(\tau+i\lambda)n_{l-\sigma}} n_{l\sigma} \rangle \quad (26)$$

We have

$$\begin{aligned}
 \langle e^{in_{k-\sigma}} (1 - n_{k\sigma}) \rangle &= (1-n) + \frac{n}{2} e^{\beta\xi} + \langle n_{k-\sigma} n_{k\sigma} \rangle (1 - e^{\beta\xi}) \\
 \langle e^{-in_{k-\sigma}} n_{k\sigma} \rangle &= \frac{n}{2} - \langle n_{k-\sigma} n_{k\sigma} \rangle (1 - e^{-\beta\xi})
 \end{aligned}
 \tag{27}$$

Using Eq. (15) we can obtain the explicit form of Eq. (27). Inserting these results in Eq. (25) we get for the dc conductivity

$$\begin{aligned}
 \sigma_{dc} &= \lim_{\omega \rightarrow 0} \sigma(\omega) \\
 &= \pi \sigma_0 \beta \delta(\omega) \frac{n}{(1 + e^{\beta\xi})^2} [e^{\beta\xi} + (1-n)e^{2\beta\xi}]
 \end{aligned}
 \tag{28}$$

with $\xi = (T_0 + U - \mu)$ and $\sigma_0 = ge^2 a^2 \hbar t^2$. Using the value of μ given by Eq. (8) we can write the dc conductivity as

$$\sigma_{dc}(\beta, n) = \pi \sigma_0 \beta \frac{n(n-2) \delta(\omega)}{[1 + \sqrt{(1-n)^2 - n(n-2)} e^{-\beta U}]^2} [(1-n)^2 + \sqrt{(1-n)^2 - n(n-2)} e^{-\beta U}]
 \tag{29}$$

We note some interesting aspects of Eq. (29). First, for $n=1$ the equation agrees with a result first obtained by Bari and Kaplan¹¹. Also, the equation predicts correctly zero conductivity for $n=0$ and $n=2$, as it must be. It is invariant under the substitution $n \rightarrow (2-n)$ reflecting the particle-hole symmetry⁴. Finally we observe that for a given temperature the shape of the conductivity curve (in our approximation) depends on n and U only. t simply fixes the scale.

5. APPLICATION TO THE CHARGE TRANSFER SALTS

The conductivity of NMP-TCNQ (for which $n=1$) has been measured by Epstein²⁰. For temperatures in the range $50^\circ\text{K} < T < 400^\circ\text{K}$ he found

$$\sigma(T) = \sigma_0 T^{-\alpha} e^{-\Delta/T}
 \tag{30}$$

with σ_0^{-1} , a and Δ constants. Recalling that under the relaxation time approximation $\delta(\omega) \rightarrow \tau_e/\pi$ where τ_e is temperature dependent we see that our Eq.(29) predicts the result in Eq.(30) if we take

$$\tau_e(T) = T^{(1-\alpha)} \quad (31)$$

and $A = U/2$. α has been found to be between 3 and 4. Now, the recent discovery of spin waves in TTF-TCNQ has been interpreted as evidence for the presence of strong Coulomb interactions in this charge transfer salt. Assuming conductivity in one stack only, Torrance et al.⁹ have shown that the experimental data are compatible with the single Hubbard model if the charge transfer is $n = 0.59$, corresponding⁶ to $U/t \gg 1$. We may then expect Eq. (29) to be applicable to this material also. Unfortunately in this case [assuming a simple temperature dependence for τ_e as in Eq.(31)] we have the prediction of a conductivity which approaches infinity at low temperatures. This is at variance with the experimental data²¹ which show that the conductivity starts to diminish below 55°K. This is also the case for the TSeF-TCNQ. In fact TTF-TCNQ exhibit the most unusual properties presenting phase transitions at 38°, 49° and 54°K. The explanations of these properties are not known at present time²².

6. CONCLUSIONS

It was our aim in this paper to obtain a simple formula for the conductivity of strong correlated systems, as a function of the electron concentration and temperature. It was expected that with the aid of the conductivity measurements we could distinguish between different values of the charge transfer in the quasi unidimensional materials like TTF-TCNQ. This expectation has not been realized. Eq. (29) cannot distinguish very much values of n in the range $0.40 < n < 0.60$. Even worse is the fact that with the exception of MMP-TCNQ (for which $n = 1$), the single Hubbard model predicts infinity growing conductivity for TTF-TCNQ at low temperatures which is at variance with the experimental data. This is an interesting point since the single Hubbard model seems to predict quite well the spin waves and the susceptibility in this material. As a final comment we must say that the δ -function peak obtained in Eq. (29) is

due to the fact that no dissipation mechanism was included in the model studied.

A finite conductivity can be obtained taking into account the electron-phonon interaction^{23,24}. Starting with the Hamiltonian

$$H = \sum_{i,j,\sigma} t_{ij} c_{i\sigma}^{\dagger} c_{j\sigma} + U \sum_i n_{i\uparrow} n_{i\downarrow} + \sum_{\vec{q}} \omega_{\vec{q}} b_{\vec{q}}^{\dagger} b_{\vec{q}} + \sum_{\vec{q},i,\sigma} A_{\vec{q}} e^{i \cdot \vec{q} \cdot \vec{R}_i} n_{i\sigma} (b_{\vec{q}} + b_{-\vec{q}}^{\dagger}) - \mu \sum_i n_{i\sigma} \quad (32)$$

where the symbols have the usual meaning a finite conductivity can be obtained. The structure is the same as Eq. (29) with a temperature dependent relaxation time, which for $n=1$ is of the form suggested in Eq. (31). We will investigate this problem in a future publication.

APPENDIX

Precise definitions are given for the real and imaginary times Green's functions used in this paper.

The causal retarded and advanced Green's functions are defined by.

$$G_{r,a}(t, t') = \pm i\theta[\pm t - t'] \langle \{ c_{i\sigma}(t) c_{j\sigma}^{\dagger}(t') \} \rangle \equiv \langle \langle c_{i\sigma}(t); c_{j\sigma}^{\dagger}(t') \rangle \rangle_{r,a} \quad (A-1)$$

where $\{ , \}$ is the anticommutator and $\langle \rangle$ indicates the average over a grand canonical ensemble at temperature T. We define for real E the Fourier transforms

$$\langle \langle c_{j\sigma}; c_{j\sigma}^{\dagger} \rangle \rangle_E^{r,a} = 1/2\pi \int_{-\infty}^{+\infty} dt e^{iEt} \langle \langle c_{i\sigma}(t); c_{j\sigma}^{\dagger}(0) \rangle \rangle_{r,a} \quad (A-2)$$

The analytic continuation of these functions into the complex energy plane will be denoted by $\Gamma_{ij}^{\sigma\sigma'}(E)$.

The imaginary time **Green's** functions is defined as

$$G_{ij}^{\sigma\sigma'}(t, t') = - \langle T_t | \psi_{i\sigma}(t) \psi_{j\sigma'}^+(t') | \rangle \quad (\text{A-3})$$

where T is the **time-ordering** operator $\psi_{i\sigma}$ and $\psi_{i\sigma}^+$ are imaginary time **annihilation** and **creation** operators defined by

$$\begin{aligned} \psi_{i\sigma}(t) &= e^{Kt} c_{i\sigma} e^{-Kt} \\ \psi_{i\sigma}^+(t) &= e^{Kt} c_{i\sigma}^+ e^{-Kt} \end{aligned} \quad (\text{A-4})$$

where

$$K = H - \mu N \quad (\text{A-5})$$

is the grand canonical Hamiltonian, μ the **chemical potential**, and N the **particle number** operator. The Fourier transform of (A-3) is defined by

$$G(t) = 1/k_B t \sum_{\ell=0}^{\infty} e^{i\omega_{\ell} t} G(\omega_{\ell}) \quad (\text{A-6})$$

where $\omega_{\ell} = \pi(2\ell + 1)/k_B T$ is the **fermion frequency**.

REFERENCES

1. David Adler, Solid State Phys. **vol.** 21, 1 (1968).
2. J. Hubbard, Proc. Roy. Soc. **A276**, 238 (1963).
3. Waldir A. Rodrigues Jr, Ellen Yoffa and David Adler. The Hubbard **Hamiltonian** revisited (MIT Preprint 1978).
4. Elliot H. Lieb and F.Y. Wu Phys. Rev. Letters, 20, 1445 (1968).
5. A.A. Ovchinnikov, Sov. Phys. JETP, 30, 1160 (1970).
6. Cornelius F. Coll, III, Phys. Rev. **B9**, 2150 (1974).
7. H. Shibus, Phys. Rev. **B6**, 930 (1972).
8. J.B. Toirrance, Y. Tombiewicz, B.D. Silverman, to be published, Phys. Rev. B. (15 April 1977).
9. J.B. Toirrance, H.A. Mook, C.R. Watson, Jr., Spin Waves in an Organic Metal: TTF-TCNQ (IBM preprint - 1976).
10. E.J. Yoffa and D. Adler, Phys. Rev. **B12**, 2260 (1975).
11. E.J. Yoffa and D. Adler, to be published in Phys. Rev. B.

12. R.A. Bari and T.A. Kaplan, Phys. Rev. *B6*, 4623(1972).
13. R.A. Bari, Phys. Rev. *B10*, 1560 (1974).
14. R.A. Bari, Phys. Rev. *B9*, 4329 (1974).
15. K. Kubo, Journal.of the Phys. Soc. of Japan, 31, 30 (1971).
16. S.K. Lyo, Phys. Rev. *B14*, 2335 (1976).
17. D.N. Zubarev, Soviet Phys. USPEKAI, 3, 320 (1960).
18. A.L. Fetter and J.D. Walecka, *Quantum Theory of Many Particle Systems* (McGraw-Hill, 1971).
19. R. Kubo, J. Phys. Soc. Japan 28, 1402 (1957).
20. A.J. Epstein, 1977 March Meeting of the American Physical Society, Bulletin of the Am. Phys. Soc. 22, 422 (1977).
21. J.R. Cooper, D. Jerome, S. Etemad, 1977 March Meeting of the American Physical Society, Bulletin of the Am. Phys. Soc. 22, 287 (1977).
22. J. Ehlers, K. Hepp, R. Kippenhahn, HA. Weidenmüller, J.Zittartz (editor~), *Organic Conductors and Semiconductors* (Springerverlag 1977).
23. R.A. Bari, Phys. Rev. *B3*, 2662 (1971).
24. P.K. George, *Physica* 49, 278 (1970).