Conductivity of interacting spinless fermion systems via the high dimensional approach

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Abstract

Spinless fermions with repulsion are treated non-perturbatively by classifying the diagrams of the generating functional $\Phi$ in powers of the inverse lattice dimension $1/d$. The equations derived from the first two orders are evaluated on the one- and on the two-particle level. The order parameter of the AB-charge density wave (AB-CDW) occurring at larger interaction is calculated in $d = 3$. The Bethe-Salpeter equation is evaluated for the conductivity $\sigma(\omega)$ which is found to have two peaks within the energy gap $2\Delta$ in the AB-CDW: a remnant of the Drude peak and an excitonic resonance. Unexpectedly, $\sigma_{DC}$ does not vanish for $T \rightarrow 0$. 
The limit of infinite dimensions $d \to \infty$ for itinerant fermion systems \cite{1, 2} has proven very useful for the understanding of strongly interacting electron systems \cite{3}. The research focuses on one-particle properties in the strict limit $d = \infty$. There exist also some results on transport properties \cite{4, 5}. The present contribution extends the knowledge on the AC- and DC-conductivity including $1/d$-corrections in the model of spinless fermions with repulsive interaction. The results cover and the non-symmetry broken (homogeneous) phase and the AB-CDW occurring on bipartite lattices. The techniques used in the description of the latter are certainly transferable to other symmetry broken phases in related models.

The Hamiltonian of the spinless fermion model at half-filling ($n = 0.5$) is given in second quantisation

$$\hat{H} = -\frac{t}{\sqrt{2d}} \sum_{<i,j>} \hat{c}_i^+ \hat{c}_j + \frac{U}{4d} \sum_{<i,j>} \hat{n}_i \hat{n}_j - \frac{U}{2} \sum_i \hat{n}_i. \quad (1)$$

Scaling with the inverse dimension $1/d$ of the considered hypercubic lattice is performed to ensure the continuity of the limit $d \to \infty$. The model is appropriate for the description of strongly polarised fermions where the band of one of the spin species is completely filled (for references on the model see ref. \cite{6}). In the strict limit $d = \infty$ the perturbation series in the interaction can be resummed since only the Hartree terms contribute \cite{2}. This transparent situation provides a good starting point for the calculation of $1/d$-corrections \cite{6, 7}. In view of the preservation of conservation laws, it is, however, not trivial to include $1/d$-corrections. At least for the considered case it was shown in detail that the formalism of Baym/Kadanoff \cite{8} avoids inconsistencies \cite{7}. In this formalism the self-energy $\Sigma(1; 2)$ (1 being shorthand for ($i_1, \tau_1$) etc.) and the kernel of the Bethe-Salpeter equation $\Xi(1, 2; 3, 4)$ are derived from a generating functional $\Phi$ according to $\Sigma(1; 2) = \delta \Phi / \delta G(2; 1)$ and $\Xi(1, 2; 3, 4) = \delta \Sigma(1; 3) / \delta G(2; 4)$. The exact $\Phi$-functional is the sum of all closed skeleton diagrams.

To obtain an expansion in the inverse dimension $1/d$ the diagrams belonging to $\Phi$ are classified in powers of $1/d$. Truncation after the desired order yields an approximate $\Phi_N$ and hence an approximation for $\Sigma$ and $\Xi$. In the present work the two leading orders $\mathcal{O}(1)$ and $\mathcal{O}(1/d)$ are kept. The resulting $\Phi_N$ is shown in Fig. 1. Halvorsen, Uhrig and Czycholl set up and evaluated the ensuing system of self-consistent equations \cite{6}. Here it is sufficient to know that the self-energy consists of two site-diagonal terms $\Sigma^H_i$ (Hartree) and $\Sigma^C_i$ (local correlation) and the Fock-term $\Sigma^F$ which links adjacent sites and renormalises thereby the hopping $t \to t':= t - \Sigma^F \sqrt{2d}$. In the homogeneous phase the local self-energy is constant. In the AB-CDW the local self-energy alternates from site to site. The order parameter $b$ of this phase is the particle density difference between a specific site and the average density $b := |\langle \hat{n}_i \rangle - n|$, i.e. the density is above (below) average on the sites on sublattice A (B) of the bipartite hypercubic lattice. In Fig. 2 the generic behaviour of $b(T)$ is shown and compared to the results of a Hartree- and a Hartree-Fock calculation. The inclusion of $1/d$ terms does not change the qualitative form of the curve. The quantitative changes are also quite moderate. From this and from a quantitative comparison with the exact results in $d = 1$ \cite{6} one can deduce that the $1/d$ expansion yields a good approximation in $d = 3$.  

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At \( n = 0.5 \) the spontaneous symmetry breaking implies an energy gap \( 2\Delta \) at the Fermi level. This gap is lowered by the \( 1/d \) terms as is the order parameter \( b \) in Fig. 2. At \( T = 0 \) the imaginary part of the local self-energy displays a gap which is exactly three times \( 2\Delta \). This stems from the fact that due to the gap in the one-particle spectrum a minimum energy of \( 6\Delta \) is required for an inelastic scattering process. This phenomenon implies the existence of undamped quasi-particles for energies in the interval \( (\Delta, 3\Delta) \) measured from the Fermi level \( \nu/\lambda \). They lead to interesting effects in the conductivity (see below).

To calculate two-particle quantities the Bethe-Salpeter equation with the kernel \( \Xi \) must be solved which is a very complicated task. For the conductivity \( \sigma(\omega) = \sigma_1(\omega) + \sigma_2(\omega) \), the current-current response function \( \chi^J(\omega) \) must be known since \( \sigma_1 = -i(\hat{T})/(\omega d) \) and \( \sigma_2 = -\chi^J/\omega \) holds ((\( \hat{T} \)) is the kinetic energy). Due to the odd parity of the current vertex \( J \) in k-space only a part of the Bethe-Salpeter equation contributes to \( \chi^J \). This leads in the present case to a tractable geometric series for \( \chi^J \) which is shown in Fig. 3. The vertical interaction lines result from the Fock diagram which is shown in Fig. 3. The series in Fig. 3 leads to \( \chi^J = \chi_0^J/(1 + U\chi_0^J/2) \) if \( \chi_0^J \) is defined as the simple bubble of dressed propagators (first diagram in Fig. 3). Explicitly, \( \chi_0^J \) is given in the homogeneous phase by

\[
\chi_0^J(i\zeta_m) = \frac{2T}{d} \sum_{\omega_\nu - \zeta_m} \int_{BZ} \frac{\sin^2(k_1)}{(w_\nu - t'\varepsilon(k))(w_\lambda - t'\varepsilon(k))(2\pi)^d} dk^d
\]

(2)

where \( w_{\nu/\lambda} := i\zeta_{\nu/\lambda} - \Sigma(i\zeta_{\nu/\lambda}) \) with roman indices for bosonic Matsubara-frequencies and greek indices for fermionic. The dispersion \( \varepsilon(k) = t\sqrt{2/d} \sum_{i=1}^d \cos(k_i) \). The sum over the \( k \)-vectors in the Brillouin-zone BZ can be carried out with a density \( \rho^0_L(\omega) := \int_{BZ} (\sin k_1)^2 \delta(\omega - \varepsilon(k)) dk^d/(2\pi)^d \). If \( \rho^0(\omega) \) is the usual DOS one may find \( \rho^0(\omega) \) from the relation \( \rho^0(\omega) = -(2/\omega)\partial\rho^0_L/\partial \omega \). In the AB-CDW, \( \chi^J \) is the \((1,1)\)-coefficient of a \( 2 \times 2 \) matrix \( -2(1 + U\Delta/2)/U \) since already the one-particle propagators are \( 2 \times 2 \) matrices. The quasi-particles at wave vector \( k \) couple with those at \( k + Q \) where \( Q = (\pi, \pi, \ldots, \pi)^\dagger \). The matrix \( \Delta_1 = [[A_1, A_3], [A_3, A_2]] \) is the piece of diagram between two wavy lines in Fig. 3; its coefficients are given by

\[
A_i = \frac{T}{d} \sum_{\omega_\nu - \zeta_m} \int_{-\infty}^{\infty} \frac{I_i \rho^0_L(\varepsilon) d\varepsilon}{(w_\nu^2 - (t'\varepsilon)^2 - \Delta_\nu^2)(w_\lambda^2 - (t'\varepsilon)^2 - \Delta_\lambda^2)},
\]

(3)

where \( \Delta_{\nu/\lambda} = (\Sigma_A(i\zeta_{\nu/\lambda}) - \Sigma_B(i\zeta_{\nu/\lambda}))/2 \) is half the difference of the local self-energy on the A- and the B-sublattice. The average self-energy is still denoted by \( \Sigma \). The numerators depend on \( i \): \( I_1 = w_\nu w_\lambda + (t'\varepsilon)^2 - \Delta_\nu \Delta_\lambda; I_2 = I_1 - 2(t'\varepsilon)^2 \) and \( I_3 = w_\nu \Delta_\nu - w_\lambda \Delta_\lambda \). The evaluation of (2) and (3) using the exact 3-dimensional densities \( \rho^0 \) and \( \rho^0_L \) leads to Fig. 4. In the homogeneous phase at higher \( T \) (curve a) the main feature of the real part of \( \sigma_{AC} \) is the Lorentzian Drude peak at \( \omega = 0 \). Its width is proportional to \( -\text{Im} \Sigma(\omega = 0) \), i.e. to \( T^2 \). In the AB-CDW at lower \( T \) (curve b), the energy gap is clearly visible. Yet there remains a peak of finite height at \( \omega = 0 \), of which the width, and hence the weight, tend exponentially to zero for \( T \rightarrow 0 \). The edge, where dissipation sets in
(\omega \approx 1.15), is located at 2\Delta. It is preceded by a pronounced Lorentzian which becomes a \delta-peak of finite weight at T = 0 (curve c). Mathematically, this peak results from the divergence of the geometric series in Fig. 3. Physically, the interaction lines in Fig. 3 represent a continued attraction between a quasi-particle and a quasi-hole forming an exciton. Due to the binding energy of the latter the corresponding resonance can be excited at energies a little lower than 2\Delta.

In Fig. 5 the generic result for \sigma_{DC}(T) is shown. In the homogeneous phase above \Tc \sigma_{DC} \approx 0.295 is proportional to 1/T^2. Just below \Tc, the conductivity drops because the DOS is reduced considerably due to the formation of the energy gap. Unexpectedly, however, it does not vanish at T = 0 but shows even a moderate increase. This phenomenon results from a subtle cancellation in the limit T \rightarrow 0 of an exponentially vanishing density of charge carriers (no spectral weight within the gap at T = 0) and a diverging mobility due to the suppression of scattering processes by the energy gap (infinite life time of quasi-particles) \[ \] \[ .\] In real physical systems, of course, this phenomenon will be obscured as soon as other scattering processes than the interaction driven ones (e.g. those driven by disorder) become more important. Yet in very pure systems the part of Fig. 5 at not too low temperatures should be observable.

Summarising, the feasibility of a high dimensional expansion even on the two-particle level was shown for interacting spinless fermions. Explicit results for the AC- and DC-conductivity in the homogeneous phase and in the AB-CDW were presented and discussed.

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Figure captions

**Fig. 1:** Approximate functional $\Phi_N$ exact to $O(1/d)$. The nearest-neighbour site indices $i$ and $j$ are summed. The first diagram generates the Hartree-, the second the Fock- and the third the local correlation terms.

**Fig. 2:** Order parameter $b(T)$ at $U = 2$ in $d = 3$; short dashed line: Hartree-, dashed line: Hartree-Fock-, solid line: complete $1/d$ result.

**Fig. 3:** Diagrammatic representation of the series for $\chi^{JJ}$.

**Fig. 4:** Real part of $\sigma_{AC}$ in $d = 3$ at $U = 2$. Curve a: $T = 0.300, b = 0.0$; curve b: $T = 0.155, b = 0.300$; curve c: $T = 0.0, b = 0.311$, $\delta$-peak at $\omega = 1.133$ not displayed.

**Fig. 5:** $\sigma_{DC}(T)$ in $d = 3$ at $U = 2$. 

