Quantum transport in strongly disordered crystals: Electrical conductivity with large negative vertex corrections

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Abstract. We propose a renormalization scheme of the Kubo formula for the electrical conductivity with multiple backscatterings contributing to the electron-hole irreducible vertex derived from the asymptotic limit to high spatial dimensions. We use this vertex to represent the two-particle Green function via a symmetrized Bethe-Salpeter equation in momentum space. We further utilize the dominance of a pole in the irreducible vertex to an approximate diagonalization of the Bethe-Salpeter equation and a non-perturbative representation of the electron-hole correlation function. The latter function is then used to derive a compact representation for the electrical conductivity at zero temperature without the necessity to evaluate separately the Drude term and vertex corrections. The electrical conductivity calculated in this way remains nonnegative also in the strongly disordered regime where the localization effects become significant and the negative vertex corrections in the standard Kubo formula overweight the Drude term.

1. Introduction
Fluctuations of the spatial distribution of the atomic potential gives origin to the zero-temperature resistivity of solids. In order to study in detail the impact of fluctuations of the atomic potential on charge transport it is appropriate to neglect all less important agents influencing the response of the electron gas on external electric perturbations and investigate only scatterings of free electrons on random impurities. It is usual to study the effects of impurity scatterings on an Anderson model of disordered electrons [1] with a site-independent distribution of the atomic potential. A straightforward way to investigate this model is to use a perturbation (diagrammatic) expansion in the random atomic potential. Nontrivial and physically interesting results can be, however, reached only via non-perturbative approaches. The most reliable non-perturbative method of describing the effects of disorder on one-electron functions is a mean-field, coherent-potential approximation (CPA) [2]. This approximation is, however, not so reliable in the strong-disorder limit for transport properties determined by response functions derived from the two-particle Green function. Due to even symmetry of the two-particle CPA vertex, there are no vertex corrections to the electrical conductivity in single-band models. There is hence no sign of possible vanishing of diffusion predicted by Anderson [1].

It is very difficult to approach Anderson localization in approximate treatments of transport properties, since the vertex corrections to the Drude (CPA) conductivity have generally
negative sign. They actually precisely compensate the Drude term in the localized phase. Standard approximate treatments cannot guarantee non-negativity of the total conductivity calculated from the Kubo formula. If we define the two-particle vertex from the two-particle Green function $G_{kk'}^{ab}(q; E_F + \omega + i a^0, E_F + i b^0)$ from an equation $G_{kk'}^{ab}(q) = G_k^a G_{k-q}^b \left[ \delta(k-k') + \Gamma_{kk'}^{ab}(q) G_k^a G_{k'+q}^b \right]$, the conductivity in direction $\alpha$ can be written as a sum $\sigma_{\alpha\alpha} = \sigma_{\alpha\alpha}^{(0)} + \Delta \sigma_{\alpha\alpha}$ where

$$\sigma_{\alpha\alpha}^{(0)} = \frac{e^2}{\pi N} \sum_k |v_\alpha(k)|^2 |G^{R}(k)|^2$$

is the one-electron Drude (mean-field) contribution and

$$\Delta \sigma_{\alpha\alpha} = \frac{e^2}{2\pi N^2} \sum_{kk'} v_\alpha(k) v_\alpha(k') \left\{ |G_{kk'}^{R}|^2 |\Delta \Gamma_{kk'}^{AR}|^2 - \Re \left[ \left( G_{kk'}^{R} \right)^2 \Delta \Gamma_{kk'}^{RR} \left( G_{kk'}^{R} \right)^2 \right] \right\} .$$

are vertex corrections due to the odd part $\Delta \Gamma$ of the two-particle vertex $\Gamma$. We denoted $k, k'$ the incoming and outgoing electron momenta, $q$ the difference between the incoming momenta of the two electrons and $\omega$ is the difference in their energies. We usually suppress the energy variables in Green functions, since they are not dynamical and use in general expressions abbreviation $a, b$ for $\pm 1 \ (R, A)$ according to the way the real frequencies of the electron and hole are approached in the complex plane, upper and lower respectively.

We use Bethe-Salpeter equations and the limit to high spatial dimensions to avoid the decoupling of the total conductivity into the one-electron part and vertex corrections so that non-negativity of the conductivity can be guaranteed even in the vicinity of the Anderson localization transition.

2. Electrical conductivity from a symmetric Bethe-Salpeter equation

We redefine two-particle vertices in momentum space by multiplying them from right and left by one-electron propagators

$$\tilde{X}_{kk'}^{ab}(q) = G_k^a X_{kk'}^{ab}(q) G_{k'+q}^b$$

so that we can write Bethe-Salpeter equations in a symmetric way with simple matrix multiplication in momentum space

$$\tilde{\Gamma}_{kk'}^{ab}(q) = \tilde{X}_{kk'}^{ab}(q) + \frac{1}{N} \sum_{kk''} \tilde{X}_{kk''}^{ab}(q) \tilde{\Gamma}_{kk''k'}^{ab}(q) .$$

Analogously to the Bethe-Salpeter equation for vertex $\Gamma$ we obtain a symmetrized Berthe-Salpeter equation for the full two-particle Green function the solution of which we formally represent as

$$G_{kk'}^{ab}(q) = G_{k+q}^b \left[ 1 - \hat{\Lambda}_{kk'}^{ab}(q) \right]^{-1} G_k^a ,$$

where $*$ stands for the appropriate matrix multiplication in the $eh$ scattering channel. This representation of the two-particle Green function can then be used to derive a non-perturbative representation of the electrical conductivity that is free of the decomposition into the Drude term and vertex corrections. We obtain for the static optical isotropic conductivity at zero temperature

$$\sigma_{\alpha\beta} = \frac{e^2}{2\pi N^2} \sum_{kk'} v_\alpha(k) \left\{ G_k^A \left[ 1 - \hat{\Lambda}_{kk'}^{AR} \right]^{-1} G_{k'}^R - \Re \left( G_k^A \left[ 1 - \hat{\Lambda}_{kk'}^{RR} \right]^{-1} G_{k'}^R \right) \right\} v_\beta(k') .$$
It is clear that only the odd part of the irreducible vertex $\Lambda^{ab}$ contributes in a nontrivial way (beyond Drude) to the electrical conductivity. One can use numerical techniques to find the inverse operators from a known irreducible vertex $\Lambda^{ab}$. We use a simpler way to assess the leading vertex corrections to the mean-field conductivity.

3. Expansion around mean field

As fairly known, the mean-field equilibrium solution (CPA) with momentum-independent self-energy $\Sigma(z)$ leads to a local irreducible vertex $\lambda(z_1, z_2) = (\Sigma(z_1) - \Sigma(z_2)) / (G(z_1) - G(z_2))$ as given by the Ward identity [3]. We hence have to go beyond the equilibrium mean-field solution and evaluate non-local corrections to the multiple single-site scatterings when calculating transport properties. The expansion beyond the mean field solution is controlled by the nonlocal part of the mean-field propagator

$$\tilde{G}(k, \zeta) = \frac{1}{\zeta - \epsilon(k)} - \int \frac{d\epsilon(\epsilon)}{\zeta - \epsilon}$$

with $\zeta = z - \Sigma(z)$. The leading-order contributions to the non-local part of the irreducible vertex $\epsilon h \lambda$ comes from multiple electron-electron scatterings (Cooperons). They can be summed explicitly [4]

$$\lambda^{ab}_{kk'}(q) = \lambda^{ab} \left[ 1 + \frac{\lambda^{ab} \chi^{ab}(k + k' + q)}{1 - \lambda^{ab} \chi^{ab}(k + k' + q)} \right]$$

where $\chi(\zeta, \zeta'; q) = N^{-1} \sum_k \tilde{G}(k, \zeta) \tilde{G}(k + q, \zeta')$ is the two-particle bubble with off-diagonal mean-field propagators $G(k, \zeta)$ while $\chi$ is the bubble with the full mean-field one-electron propagators $G(k, \zeta)$. It is worth noting that $(\epsilon h) \lambda^{RA}$ contains a pole at the Fermi energy [5]. Due to the Velický–Ward identity we have $\lambda^{RA} \chi^{RA}(0) = 1$. Vertex from Eq. (8) is a leading-order contribution to the irreducible vertex in the $\epsilon h$ channel in high spatial dimensions justifying the mean-field approach [6].

We use the irreducible vertex from Eq. (8) in the evaluation of the electrical conductivity in Eq.(6). We then have to invert a matrix $L^{-1}_{kk'}(q) = \delta_{kk'}^0 - \lambda G_k G_{k+q} S(k + k' + q)$ where we denoted $S(Q) = \lambda \chi(Q) / [1 - \lambda \chi(Q)]$. Since the dominant contribution to momentum summations comes from the vicinity of the pole in $S(0)$, that is for $k + k' + q \approx 0$, we can replace the product of the one-electron propagators $G_k G_{k+q}$ in $L^{-1}_{kk'}(q)$ by an average $N^{-1} \sum_k G_k G_{k'}$ in this matrix, since we sum over the intermediate fermionic momenta during matrix inversion. This simplifying approximation allows us to find an analytic expression for a modified matrix $L^{-1}_{kk'}(q) \approx \delta_{kk'} - \lambda \chi(0) S(k + k' + q)$. To calculate the inverse we use a Fourier transform defined in a $d$-dimensional momentum space $\tilde{f}(x) = \int d^d x e^{i x \cdot \xi} f(x)$. Matrix inversion is thereby transformed to algebraic one and we obtain

$$L^{-1}_{kk'}(q) = \int \frac{d^dx}{(2\pi)^d} \left[ \frac{e^{-i(k-k') \cdot x} \lambda \chi(0) S(-x) S(x)}{1 - \lambda^2 \chi(0)^2 S(x) S(-x)} \right]$$

We further introduce Fourier transforms of velocities as $\tilde{v} G(x) = \int d^d k v(k) G_k e^{i k \cdot x}$ so that we reach a representation of the electrical conductivity containing vertex corrections to the mean-field Drude conductivity in a form guaranteeing its non-negativity

$$\sigma = \frac{e^2}{2\pi} \int \frac{d^d x}{(2\pi)^d} \left[ \tilde{v} G^A(x) \tilde{v} G^R(-x) \lambda \chi(0) S^A S^R(0) \right] - \Re \left( \frac{\tilde{v} G^R(x) \tilde{v} G^R(-x)}{1 + \lambda^{AR} \chi^{AR}(0) S^{AR}(0)} \right) \equiv \sigma^{AR} - \Re \sigma^{RR}.$$  \hspace{1cm} (10)

Note that $\tilde{v} G(x) = -\tilde{v} G(-x)$ while $\tilde{S}(x) = \tilde{S}(-x)$. It is the first term on the right-hand side of Eq. (10) that is dominant within the band with non-zero imaginary part of the self-energy and $\sigma^{AR} \geq |\sigma^{RR}| \geq 0$. 

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4. Results and discussion

We use expression Eq. (10) and calculate the conductivity for a binary alloy on a simple-cubic lattice. We resort to the mean-field approximation (CPA) of the one-electron self-energy. One finds a split-band transition in the spectral function with diverging imaginary part of the self-energy at a disorder strength $\Delta \approx 2.45t$, where $t$ is the nearest-neighbor hopping amplitude. Vertex corrections to the electrical conductivity are strong near this transition and their separation from the symmetric Drude term becomes unreliable, leading to negative values of the conductivity. We plotted in Fig. 1 the Drude conductivity, Drude conductivity with the first vertex correction and the approximate conductivity from Eq. (10). We can see that close to the band edge the vertex corrections indeed overturn the sign of the conductivity and separate evaluation of vertex corrections becomes unreliable. Our non-perturbative formula does not show any unphysical behavior and the conductivity remains non-negative within the whole energy band. We also plotted in Fig. 2 contributions to the full conductivity from its two parts $\sigma^{AR}$ and $\sigma^{RR}$. We can see that $\sigma^{RR} \leq 0$ near split band but its absolute value does not go over that of $\sigma^{AR}$. Note that $\Im \Sigma(0) = -\infty$ at the inner split-band edge $\Delta \approx 2.45t$, that is why $\sigma^{AR} = -\sigma^{RR} = 0$. At the outer band edges where $\Im \Sigma(0) = 0$ we have $\sigma^{AR} = \sigma^{RR} = \infty$.

To conclude, we presented an approximate non-perturbative expression for the electrical conductivity with leading-order vertex corrections guaranteeing its non-negativity in the entire energy region as well as for all disorder strengths. It can hence be used to extend the standard mean-field one-electron approximation by including leading two-particle vertex corrections to the electrical conductivity without breaking the fundamental physical laws.

References

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Figure 1. Electrical conductivity on a single-cubic lattice with local mean-field self-energy. Drude conductivity $\sigma^{(0)}$, with vertex corrections $\Delta \sigma$ and conductivity $\sigma_A$ from Eq. (10) compared.

Figure 2. Contributions to the conductivity from its $AR$ and $RR$ parts as decomposed in Eq. (10). The more inside the band the more dominant $\sigma^{AR}$ becomes.