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Theories of impurity resistivity in two dimensions

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Abstract. All important theories of impurity resistivity in three dimensions each give one of two results. All results are obtained without any implicit inclusion of electron–electron scattering. The electron–electron scattering has an indirect effect on the impurity resistivity in that it affects the distribution function for the carriers. Result number one is found in the limit of no electron–electron scattering while the second result is found from theories where the basic assumption is that the electrons are thermalized in their centre-of-mass system, i.e. very strong electron–electron scattering. Thus the two results can be viewed as the upper and lower limits of the result of a more elaborate theory including electron–electron scattering. In the present work we study the corresponding upper and lower limits for impurity scattering in a two-dimensional system. Numerical results for general temperatures are presented for δ-doped GaAs. Analytical expressions are given for the low- and high-temperature limits of the resistivity.

1. Introduction

The present work is an extension to two dimensions (2D) of our earlier discussion [1, 2] of the basic theory of impurity resistivity in three dimensions (3D). This discussion was inspired by the recent renewed interest in impurity resistivity sparked by the discovery [3–5] that the force-balance [6–12] type of theories have the same basic problems as the resistivity formulations [13–17] were found [18] to have two decades ago.

We will not go into any great details here but only summarize the important facts for the 3D case. All important theories of impurity resistivity give one of two results. The results are different for finite temperatures but merge for lower temperatures. The first is

$$\sigma = (ne^2/m^*)\langle\tau(k)\rangle \tag{1}$$

and the second is

$$\rho = (m^*/ne^2)\langle 1/\tau(k)\rangle \tag{2}$$

where in 3D the angle brackets stand for the following averaging procedure

$$\langle A(k)\rangle = -\frac{4}{3n}\int\frac{\mathrm{d}^3k}{(2\pi)^3}\frac{\partial f^0(k)}{\partial\epsilon_k}\epsilon_k A(k). \tag{3}$$

The Kubo (K) formula for the current–current correlation function obtained with diagrammatic perturbation theory (to infinite order) and the solution of the

Boltzmann equation (BE), both give result number one while result number two is obtained from the resistivity formulations (to lowest order), the force-balance methods (FB), the energy-loss method (EL) [19], the generalized Drude approach (GDA) [20] and the lowest-order variational solution of the Boltzmann equation (BEV) [21]. Result number two is also obtained from the Kubo formula for the force–force correlation function.

All results are obtained without any explicit inclusion of electron–electron (e–e) scattering. This scattering mechanism does not contribute directly to the resistivity in the case of an isotropic one-component carrier system. However, it contributes indirectly in that it changes the distribution function for the carriers. This in turn modifies the impurity scattering. The first result is correct in the absence of e–e scattering while the second is correct in the limit of very strong e–e scattering (which leads to complete thermalization in the centre-of-mass system for the carriers). A correct treatment of the conductivity-, resistivity- and force-balance formulations in the presence of e–e scattering (or any other inelastic scattering mechanism that strives towards a thermalization of the carriers) leads to the same result, somewhere in between the above. Thus, the two results can be regarded as the lower and upper limits, respectively, of the correct impurity resistivity.

In the present work we determine the corresponding results for a 2D system. The numerical results are presented for a system that can be regarded as an idealization for an n-type δ-doped layer in GaAs; the shallow donors are assumed to be distributed at random within the doping plane; the finite extension of the electron wavefunction perpendicular to the plane is neglected; only one quantized level is occupied and effects from interband transitions are neglected; we assume a neutral layer, i.e. one free electron per donor in the layer.

We extract the first result from the standard semi-classical Boltzmann equation and then we use the generalized Drude approach (GDA) to obtain the second result. The derivations together with the numerical results are presented in section 2. We introduce the generalized Thomas–Fermi screening in 2D in section 3 in order to simplify the calculations and in section 4 we study explicitly the high- and low-temperature behaviour of the two results. Finally we give a summary and conclusions in section 5.

2. Impurity resistivity in two dimensions

The calculations are, as mentioned above, performed for heavily n-doped GaAs under the assumption that the donors are randomly distributed and that the impurity potential can be approximated by a pure Coulomb potential. The background dielectric constant K is set to 13.0 and we have used the value 0.06 m_e for the effective mass m^*.

The Boltzmann equation implies that for the steady-state condition the occupation number for state k is unchanged with time, i.e.

$$[\partial f(k)/\partial t]_{\text{scatt.}} + [\partial f(k)/\partial t]_{\text{field}} = 0. \tag{4}$$

The first term is the *collision term* and the second term is referred to as the *drift term*. If we only have impurity scattering we can rewrite the expression as

$$\frac{4\pi e^4 m^* n}{\hbar^3 K^2} \int d^2q \frac{[f(k) - f(k+q)]\delta[q^2 + 2kq\cos(k,q)]}{q^2\epsilon^2(q,0)} - \frac{eE}{\hbar}\frac{\partial f(k)}{\partial k} = 0. \tag{5}$$

The relaxation time $\tau(\mathbf{k})$ can be defined by

$$f(\mathbf{k}) = f^0\left(\mathbf{k} + \frac{e\tau(\mathbf{k})\mathbf{E}}{\hbar}\right) \tag{6}$$

where f^0 is the Fermi distribution function. Linearizing the expression and keeping the lowest-order terms gives

$$\frac{4\pi e^4 m^* n}{\hbar^3 K^2}\frac{e\mathbf{E}}{\hbar}\tau(\mathbf{k})\frac{\partial f^0(\mathbf{k})}{\partial\epsilon_k}\frac{\partial\epsilon_k}{\partial\mathbf{k}}\int \mathrm{d}^2q \frac{[1-\cos(\mathbf{k},\mathbf{k}+\mathbf{q})]\delta[q^2+2kq\cos(\mathbf{k},\mathbf{q})]}{q^2\epsilon^2(q,0)} - \frac{e\mathbf{E}}{\hbar}\frac{\partial f^0(\mathbf{k})}{\partial\epsilon_k}\frac{\partial\epsilon_k}{\partial\mathbf{k}} = 0. \tag{7}$$

The relaxation time can thus be identified as

$$\frac{1}{\tau(\mathbf{k})} = \frac{4\pi e^4 m^* n}{\hbar^3 K^2}\int \mathrm{d}^2q \frac{[1-\cos(\mathbf{k},\mathbf{k}+\mathbf{q})]\delta[q^2+2kq\cos(\mathbf{k},\mathbf{q})]}{q^2\epsilon^2(q,0)}. \tag{8}$$

After integration over the angles this result is reduced to

$$\frac{1}{\tau(k)} = \frac{2\pi e^4 m^* n}{\hbar^3 K^2 k^3}\int_0^{2k} \mathrm{d}q \frac{1}{\epsilon^2(q,0)\sqrt{1-(q/2k)^2}}. \tag{9}$$

The resistivity is now obtained from the current density $\mathbf{j}$ which, in two dimensions, can be written as

$$\mathbf{j} = -2e\int \frac{\mathrm{d}^2k}{(2\pi)^2} f(\mathbf{k})\boldsymbol{\nu}_k \tag{10}$$

where $f(\mathbf{k})$ again is the unknown distribution function. The factor 2 is from the summation over the spins. Using equation (6) once more, linearizing and keeping the lowest-order terms gives, after some rewriting,

$$\mathbf{j} = -\frac{2e^2}{m^*}\mathbf{E}\int \frac{\mathrm{d}^2k}{(2\pi)^2}\frac{\partial f^0(k)}{\partial\epsilon}\epsilon_k\tau(k). \tag{11}$$

From $\mathbf{j} = \sigma\mathbf{E}$ we can now identify result number one with $\tau(\mathbf{k})$ given by (9) and the angle bracket standing for the following averaging procedure

$$\langle A(\mathbf{k})\rangle = -\frac{2}{n}\int \frac{\mathrm{d}^2k}{(2\pi)^2}\frac{\partial f^0(k)}{\partial\epsilon_k}\epsilon_k A(k). \tag{12}$$

This is a similar expression to the averaging procedure (3) in 3D except for a factor $\frac{2}{3}$.

In the generalized Drude approach (GDA) [20] one starts with the simple Drude expression for the dynamical conductivity

$$\sigma(\omega) = (ne^2/m^*)[1/(1/\tau - \mathrm{i}\omega)]. \tag{13}$$

The relaxation time τ is generalized to be complex-valued and frequency-dependent. If the expression is expanded for high frequencies it can be compared with a rigorous high-frequency result [22] based on the Kubo formalism and the relaxation time can thus be identified. The expression found for $\tau(\omega)$ is assumed to be valid for all frequencies, especially for zero frequency which is the limit of interest here. From (13) it is now possible to identify the resistivity, which is the inverse conductivity, as

$$\rho(\omega) = -\mathrm{i}\frac{m^*\omega}{ne^2} + \mathrm{i}\frac{1}{2nK\omega}\int_0^\infty \mathrm{d}q q^2 \left[\frac{1}{\epsilon(q,\omega)} - \frac{1}{\epsilon(q,0)}\right]. \tag{14}$$

We are here interested in the static result, which can be written as

$$\rho = \frac{1}{2nK}\int_0^\infty \mathrm{d}q q^2 \frac{1}{\epsilon^2(q,0)} \frac{\partial[\epsilon_2(q,\omega)]}{\partial\omega}\Big|_{\omega=0} \tag{15}$$

where $\epsilon_2(q,\omega)$ is the imaginary part of the dielectric function in 2D. It can be shown [23] that the GDA result can also be expressed as

$$\rho = -\frac{4\pi e^2(m^*)^2}{n\hbar^3K^2}\int \frac{\mathrm{d}^2k}{(2\pi)^2}\frac{\partial f^0(k)}{\partial\epsilon_k}\epsilon_k\frac{1}{k^3}\int_0^{2k}\mathrm{d}q\frac{1}{\epsilon^2(q,0)\sqrt{1-(q/2k)^2}}. \tag{16}$$

i.e. we have actually found result number two (2) with $1/\tau$ given by (9) and with the averaging procedure described by (12).

The dielectric function $\epsilon(q,\omega)$ in (9) and (15) cannot, to our knowledge, be obtained analytically within the random-phase approximation (RPA) in two dimensions except at zero temperature. This is different from the 3D case where the imaginary part of the dielectric function can be expressed analytically for all temperatures. We will return to the two temperature limits in section 4. In two dimensions for finite temperatures one has to calculate the dielectric function numerically from

$$\epsilon(q,\omega) = 1 + \alpha_0^R(q,\omega) \tag{17}$$

where the polarizability $\alpha(q,\omega)$ is given in the retarded form by

$$\alpha_0^R(q,\omega) = -\frac{\nu_q^{2D}}{K\hbar}2\int\frac{\mathrm{d}^2k}{(2\pi)^2}\left[\frac{n(k)-n(k+q)}{\omega-(\epsilon_{k+q}-\epsilon_k)/\hbar+\mathrm{i}\eta}\right]. \tag{18}$$

Here $n(k)$ is the Fermi occupation numbers and $\nu_q = 2\pi e^2/q$ is the Fourier transform of the Coulomb potential in two dimensions.

We present the two results in figure 1 for three different electron concentrations; 10^{10}, 10^{11} and 10^{12} cm^{-2}. Higher concentration gives lower resistivity. The full curves show the second result found from the generalized Drude approach for each electron concentration and the broken curves show the corresponding first result obtained from the semi-classical Boltzmann equation.

3. The generalized Thomas–Fermi screening

The Thomas–Fermi dielectric function is an approximation of the static dielectric function at zero temperature. We will make a more general derivation which applies

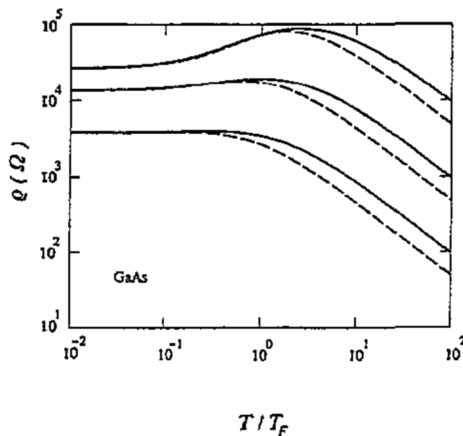

Figure 1. The resistivity as a function of T/T_F. The curves taken from the top are for the donor densities $n = 1 \times 10^{10}$, 1×10^{11} and 1×10^{12} cm^{-2}, respectively. The broken and full curves represent the limits of no e–e and very strong e–e scattering, respectively.

to finite temperatures but is still limited to zero frequencies. The Thomas–Fermi result is then found as the zero temperature limit of our expressions.

Assume that we have a potential energy $V(r,z)$ in the electron gas caused by an external charge density, $Ze\rho_i(r)\delta(z)$, and a screening charge density, $-e\rho_s(r)\delta(z)$. We let r denote the radius vector in the plane where our carriers are situated and z the perpendicular coordinate. We will be interested in the potential in the plane. Because of this it is useful to introduce the potential energy

$$U(r) = V(r,0). \tag{19}$$

The Fourier transform of Poisson's equation

$$\nabla^2 V(r,z) = (4\pi e^2/K)[Z\rho_i(r) - \rho_s(r)]\delta(z) \tag{20}$$

yields

$$V(q,k) = -(4\pi e^2/K)[Z\rho_i(q) - \rho_s(q)][1/(q^2+k^2)]. \tag{21}$$

The Fourier transform of U(r) can in turn be found from

$$U(q) = \int_{-\infty}^{\infty} \frac{\mathrm{d}k}{2\pi} V(q,k) \tag{22}$$

with together with (21) implies that

$$U(q) = -(2\pi e^2/Kq)[Z\rho_i(q) - \rho_s(q)]. \tag{23}$$

In the Thomas–Fermi approximation one assumes that the electrons behave locally as a non-interacting electron gas; the local band bottom is given by $U(r)$. The electrons are distributed in energy according to the Fermi–Dirac distribution function from the band bottom upwards; the possibility of localized states in narrow potentials is not taken into account.

If $+e\rho_0$ is the positive background charge density then the electron density to first order in the potential energy is given by

$$\rho(\boldsymbol{r}) = \rho_0 - (\partial \rho_0/\partial \mu)U(\boldsymbol{r}). \tag{24}$$

Since $\rho_s = \rho(\boldsymbol{r}) - \rho_0$ we now have

$$U(q) = -[2\pi e^2 Z \rho_i(q)/Kq\epsilon_{\mathrm{GTF}}(q)] \tag{25}$$

where in 2D

$$\epsilon_{\mathrm{GTF}}(q) = 1 + (1/q)(2\pi e^2/K)(\partial \rho_0/\partial \mu). \tag{26}$$

If we introduce the dimensionless variables

$$B = \beta E_{\mathrm{F}} \qquad M = (\mu/E_{\mathrm{F}}) \qquad A = BM = \beta\mu \tag{27}$$

and the constant

$$y = (m^* e^2/K\hbar^2 k_{\mathrm{F}}) \tag{28}$$

we can rewrite the dielectric function as

$$\epsilon_{\mathrm{GTF}}(q) = 1 + (2\pi e^2/K)(2m^*/2\pi\hbar^2)(\mathrm{d}B/\mathrm{d}A) = 1 + (2k_{\mathrm{F}}y/q)(1 - \mathrm{e}^{-B}) \tag{29}$$

where we have used the following relation for the temperature dependence of μ in 2D

$$B = \ln(1 + \mathrm{e}^{A}). \tag{30}$$

The two temperature limits are

$$\epsilon(q) = 1 + (q_{\mathrm{TF}}/q) = 1 + (2k_{\mathrm{F}}y/q) \qquad T \to 0, \text{ Thomas–Fermi (TF)} \tag{31}$$

$$\epsilon(q) = 1 + (q_{\mathrm{DH}}/q) = 1 + (2k_{\mathrm{F}}By/q) \qquad T \to \infty, \text{ Debye–Hückel (DH).} \tag{32}$$

In our derivation this dielectric function is temperature dependent. In the zero-temperature limit it becomes the ordinary Thomas–Fermi result and in the high-temperature limit it becomes the Debye–Hückel dielectric function.

The resistivity calculated with the generalized Thomas–Fermi screening is shown in figure 2 (broken curves) together with the two main results (full curves). The electron concentration used is 10^{11} cm^{-2}. Thus the simplified screening gives accurate numerical values in both the temperature limits, which also will be shown analytically in the next section. Unfortunately it fails to produce a good approximation for the full RPA in the intermediate-temperature region.

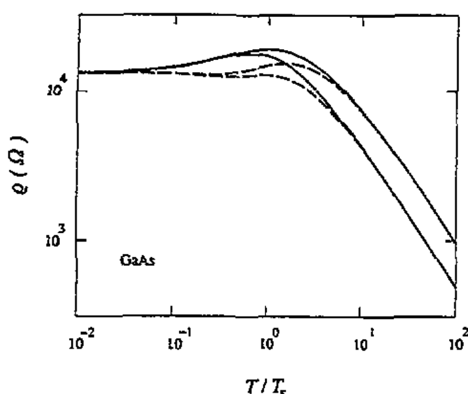

Figure 2. The resistivity as a function of T/T_F for the donor density $n = 1\times10^{11}$ cm^{-2}. The upper and lower solid curves (—) are results for no e–e and very strong e–e scattering, respectively, as defined in the text. The broken curves (- - -) are the corresponding results when the screening has been treated in the simplified generalized Thomas–Fermi approximation.

4. Temperature limits

For zero temperature it is possible to calculate the dielectric function in 2D within the full RPA and the static result is actually identical with the Thomas–Fermi expression $\epsilon(q,0) = 1 + q_{TF}/q$ with $q_{TF} = 2k_F y$ for $q < 2k_F$. This is the interval of interest here. The derivative of the imaginary part is given by

$$\frac{\partial \epsilon_2(Q,W)}{\partial W}|_{W=0} = \begin{cases} y/(Q^2\sqrt{1-Q^2}) & Q<1 \\ 0 & Q>1 \end{cases} \tag{33}$$

where $Q = q/2k_F$ and $W = \hbar\omega/4E_F$.

The zero-temperature static resistivity in the GDA is then given by (15)

$$\rho = \frac{4\pi\hbar}{e^2}\int_0^1 \mathrm{d}Q \frac{Q^2}{\sqrt{1-Q^2}(1+Q/y)^2}. \tag{34}$$

The integral can be solved to yield

$$\rho = (4\pi\hbar y^2/e^2)\,[(\pi/2) - f(1/y)] \tag{35}$$

where

$$f(x) = \frac{x}{1-x^2} + \begin{cases} 2\dfrac{1-2x^2}{(1-x^2)^{3/2}}\left[\tan^{-1}\dfrac{1+x}{\sqrt{1-x^2}} - \tan^{-1}\dfrac{x}{\sqrt{1-x^2}}\right] & x<1 \\ \dfrac{1-2x^2}{(x^2-1)^{3/2}}\ln\dfrac{(1+x-\sqrt{x^2-1})}{(1+x+\sqrt{x^2-1})} & x>1. \end{cases} \tag{36}$$

At zero temperature the averaging procedure (12) used with the Boltzmann equation solution singles out the value at the Fermi level, i.e.

$$\rho = \frac{m^*}{ne^2\langle\tau(k_F)\rangle} = \frac{m^*}{ne^2}\frac{2\pi e^4 m^* n}{\hbar^3 K^2 k_F^2}\int_0^{2k_F} \mathrm{d}q \frac{1}{\epsilon^2(q,0)\sqrt{1-(q/2k_F)^2}} \tag{37}$$

which is identical to the GDA result. The two methods thus have the same zero-temperature limit for the static resistivity within the full RPA and this result is identical with the resistivity found from the simple Thomas–Fermi screening.

It is interesting to notice that in the low-density limit or weak-scattering limit the static resistivity has an upper bound, i.e.

$$\lim_{n\to 0}\rho = \frac{4\pi\hbar}{e^2}\int_0^1 \mathrm{d}Q\,\frac{Q^2}{\sqrt{1-Q^2}} = \frac{\pi^2\hbar}{e^2} = \frac{\pi}{2}\frac{h}{e^2} \approx 4.0547\times 10^4\ \Omega. \quad (38)$$

This can also be extracted from figure 1 where the resistivity curve for the lowest electron concentration does drop significantly in the low-temperature limit. There is no corresponding decrease in the low temperature resistivity in 3D.

For high temperatures the imaginary part of the RPA dielectric function takes the form

$$\epsilon_2(Q,W) = (y\sqrt{\pi B}/4Q^2)\left\{\mathrm{e}^{-B[(W-Q^2)/Q]^2} - \mathrm{e}^{-B[(-W-Q^2)/Q]^2}\right\} \quad (39)$$

and the derivative at zero frequency is

$$(\partial\epsilon_2(Q,W)/\partial W)|_{W=0} = (y\sqrt{\pi}B^{3/2}/Q^2)\mathrm{e}^{-BQ^2}. \quad (40)$$

The real part of the RPA dielectric function can be obtained from the imaginary part through the Kramers–Kronig dispersion relations. For high temperatures, the real part approaches the Deybe–Hückel expression $\epsilon(Q,0) = 1 + Q_{\mathrm{DH}}/Q$ with $Q_{\mathrm{DH}} = By$.

In the high temperature limit the averaging procedure in equation (12) becomes

$$\langle A(k)\rangle = \frac{\beta^2\hbar^4}{2m^{*2}}\int \mathrm{d}k\ k^3\mathrm{e}^{-\beta\epsilon_k}A(k) \quad (41)$$

which implies that the high-temperature resistivity of result number one can be written as

$$\rho = (2m^{*3}/ne^2\beta^2\hbar^4)\Big/\int \mathrm{d}k\ k^3\mathrm{e}^{-\beta\epsilon_k}\tau(k) \quad (42)$$

where

$$\tau^{-1}(k) = (4\pi e^4 m^* n/\hbar^3K^2k^2)\,[(\pi/2) - f(2k/q_{\mathrm{DH}})] \quad (43)$$

and where $f(x)$ is given by (36). Since the second term vanishes for extremely high temperatures it is possible to express the very-high-temperature resistivity as

$$\rho \approx (\pi^2e^2\beta m^*/2K^2\hbar). \quad (44)$$

The generalized Drude approach gives for high temperatures

$$\rho = \frac{2\sqrt{\pi}(m^*)^2e^2B^{3/2}}{K^2\hbar^3n}\int_0^\infty \mathrm{d}Q\,\frac{Q^2\mathrm{e}^{-BQ^2}}{(Q+Q_{\mathrm{DH}})^2}. \quad (45)$$

In the extreme high-temperature limit this is reduced to

$$\rho \approx (\pi^2e^2\beta m^*/K^2\hbar)\left[1 + (4/\sqrt{\pi})B^{3/2}y\ln B^{3/2}y\right]. \quad (46)$$

If the last term is neglected we have that the generalized Drude approach gives *twice* as high a resistivity as the Boltzmann method in the high-temperature limit, independent of the electron concentration.

5. Summary and conclusions

We have studied how the results from the generalized Drude approach for impurity resistivity compare numerically with the straightforward solution of the Boltzmann equation in a 2D system. Numerical results have been presented for an n-type δ-doped layer in GaAs.

The e–e scattering has an indirect effect on the resistivity in that it changes the distribution function. In the limit of very strong e–e scattering the electrons are thermalized in their centre-of-mass system and distributed according to the Fermi–Dirac distribution function. In the other extreme limit, i.e. in the limit of no e–e scattering at all, the distribution function is different. The result from the generalized Drude approach, and from other formulations where the basic assumption is that the electrons are thermalized in their centre-of-mass system, can be viewed as the upper limit of the result of a more elaborate calculation including e–e scattering. The Boltzmann method gives the other limit. Thus the two theories give the upper and lower limits of the correct impurity resistivity when the indirect effects of e–e scattering is included. We have here determined the two limits for a 2D system.

The two results in 2D have a behaviour similar to the corresponding results in 3D—they merge for zero temperature but differ for finite temperatures. Unique to 2D is the fact that the zero-temperature resistivity has an upper bound. This gives a characteristic drop in the resistivity towards zero temperature for low donor concentrations. We have found analytical expressions for the zero-temperature static impurity resistivity and for the high-temperature limits. In the very-high-temperature limit the generalized Drude approach gives twice as high a resistivity as the Boltzmann method.

We have also found that the generalized Thomas–Fermi screening in 2D does not approximate the full RPA screening accurately in the intermediate-temperature region but the full RPA dielectric function approaches both the Thomas–Fermi expression in the low-temperature limit and the Debye–Hückel result in the high-temperature limit. This is in contrast to the 3D case where the corresponding GTF expression gives a good approximation in the whole temperature range even if the zero-temperature result is slightly different from the full RPA result.

Acknowledgment

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