The electronic thermal resistance of a metal can be expressed as

$$W_e=\lambda_e^{-1}=W_0+W_i,$$

where $W_0=\rho_0/L_0T$ is the thermal resistance caused by impurity scattering and W_i is the ideal thermal resistivity caused by phonon-electron scattering. W_i is expected to be proportional[6] to T^2. In Fig. 6 we have plotted W_i for samples 1 and 2. In both cases we have used our estimate of the lattice conductivity (Fig. 5) for sample 2 to obtain the electronic thermal conductivity. The ideal thermal resistivities are in good agreement with each other and show a T^2 temperature dependence from 14 to 25 K.

IV. SUMMARY

The thermal conductivity of high-purity thorium has been measured from liquid-helium temperatures to 200 K. Over this temperature range the thermal conductivity is in good agreement with theoretical predictions.

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Electron–Rayleigh-Wave Interaction*

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The effect of the presence of thermal Rayleigh waves on electrons is estimated. Most accessible to experiment is the case where the electrons are confined to the surface region by a magnetic field (magnetic surface level). The broadening of the level is calculated and is found to be linear in temperature in the temperature range of greatest interest.

I. INTRODUCTION

EVER since the publication of *The Theory of Sound*,[1] surface waves in elastic media have held the attention of physicists and other scientists, particularly seismologists. Only recently, however, have Rayleigh waves been produced and their attenuation been measured in crystalline solids in the ultrasonic frequency range.[2] We shall consider here the case of elastic surface waves in conducting media, where they do not seem to have been directly observed up to now.

The existence of these waves has, in the main, the same consequences for electrons as that of ordinary phonons, namely, there is a contribution to the electron's lifetime, to the electron-electron interaction, and to the effective mass. There is also, of course, a contribution to the attenuation of the elastic wave, but we shall not consider that here.

Ordinarily, these effects are negligible, which no doubt accounts for their failure to be discussed in the literature. The reason is that Rayleigh waves penetrate just about a wavelength into the solid, so that they seldom interact with the electrons. In particular, the phonon-induced effective mass and electron-electron interaction depend for their strength on high-frequency virtual phonons, so that the corresponding virtual surface phonons are not important, penetrating as they do only a few lattice constants into the solid. (If very finely divided material is used, or the effective surface-to-area ratio is greatly increased, the effect may become important, and give rise to an enhancement of the superconducting transition temperature, for example.[3])

It is thus necessary to keep the relevant electrons from alienating themselves from the surface, either by reducing the surface to volume ratio, or by supplying a force which pins the electrons against the surface. When the force has as its origin a magnetic field, the result is a localization into quasidiscrete levels confined to within about 10^{-5} cm from the surface, and known as magnetic surface levels.[4] A similar case in semiconductors leads to localization on the scale of 10^{-6} cm.[5] The primary effect of the Rayleigh wave is to contribute to the decay of these levels.

The theory of Rayleigh waves in anisotropic crystalline solids is considerably more complicated than the corresponding theory of the bulk phonon modes, and the best possible calculation would certainly require extensive computer calculations.[6] In this paper, we

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wish only to survey the general features to be anticipated and to suggest some areas where experimental investigations may bear fruit. Accordingly, we assume that the medium is isotropic in its elastic properties, and employ Rayleigh's own solution to the elasticity problem. As we shall see, the relevant wavelengths are generally long enough so that the discreteness of the lattice is of no importance.

In the general case of anisotropy, true surface waves propagating in a given direction parallel to a crystal face may or may not exist, and they may decay into the bulk regions with a complex exponent.[6] Furthermore, the so-called bulk phonons will have modified displacement vectors near the surface in the same region in which Rayleigh waves have their existence, and this modification will be reflected in the electron-phonon effects. We think that all of these complications are irrelevant insofar as the main features of the result are concerned, and probably just modify the over-all magnitude of the effect by some modest amount.

II. ELASTIC SURFACE WAVES

The displacement of the lattice in the presence of Rayleigh waves can be written

$$\mathbf{u}_{11}=iqAe^{i\mathbf{q}\cdot\mathbf{x}}e^{-pz}-kBe^{i\mathbf{q}\cdot\mathbf{x}}e^{-kz}, \tag{1a}$$

$$u_z=-pAe^{i\mathbf{q}\cdot\mathbf{x}}e^{-pz}-iqBe^{i\mathbf{q}\cdot\mathbf{x}}e^{-kz}, \tag{1b}$$

where $p=q(1-c_r^2/c_l^2)^{1/2}$, $k=q(1-c_r^2/c_t^2)^{1/2}$, and the speed of the wave c_r satisfies

$$(1-c_r^2/c_l^2)^{1/2}(1-c_r^2/c_t^2)^{1/2}=1-c_r^2/2c_t^2, \tag{2}$$

in which we have adopted the notation c_l and c_t for the longitudinal and transverse sound velocities, respectively. A typical situation would be $c_r\sim 0.9c_t$ and $c_t\sim 0.5c_l$. The dispersion relation (2) and the coefficients A and B are determined up to normalization by the requirement that the stresses vanish at the surface $z=0$. In (1), $\mathbf{q}$ is a vector parallel to the surface. The boundary condition is such that the normalization can be chosen to satisfy

$$\int d^3x\ \mathbf{u}_{\mathbf{q}\lambda}{}^*\cdot\mathbf{u}_{\mathbf{q}'\lambda'}=\delta_{\lambda\lambda'}\delta_{\mathbf{q}\mathbf{q}'}, \tag{3}$$

where $u_{\mathbf{q}\lambda}$ is the displacement associated with any of the eigenmodes either bulk or surface, of the elastic system. With this normalization the constants A and B are proportional to $(1/Sq)^{1/2}$, where S is the surface area.

As usual, phonon operators $a_{\mathbf{q}\lambda}$ are introduced by putting the displacement at $\mathbf{x}$:

$$\mathbf{u}(\mathbf{x})=\sum_{q,\lambda}\mathbf{u}_{\mathbf{q},\lambda}(\mathbf{x})\frac{a_{q\lambda}+a_{-q\lambda}{}^\dagger}{(2\rho\omega_{q\lambda}/\hbar)^{1/2}}, \tag{4}$$

where the a's obey the canonical Boson commutation relations, and ρ is the mass density of the solid. The polarization index λ runs over all phonon modes of the system, both bulk and surface in character.

III. ELECTRON–SURFACE-PHONON INTERACTION

In the presence of a lattice displacement, the local Fermi surface will dilate, deform, and rotate. Electrons passing through the region from others of differing displacement, will see a local "deformation" potential which can scatter them. The simplest aspect is that of the dilation $\nabla\cdot\mathbf{u}$ which is independent of Fermi-surface structure. This component is certainly important and we shall treat it as a prototype, since in the case of bulk phonons it has been found to lead to qualitatively correct results except for the over-all numerical factor. Anyway, Eq. (1) already represents a substantial simplification, as we have discussed.

A second contribution of different type arises because the surface becomes corrugated. A perturbation treatment of this effect[4] shows that it depends on the normal derivative of the electronic wave functions at the nominal surface, and upon the magnitude of the displacement of the surface. We assume, therefore, that the interaction Hamiltonian may be written as follows:

$$H_I=H_D+H_S, \tag{5a}$$

$$H_D=\frac{n}{N(0)}\int\psi^\dagger(\mathbf{x})\nabla\cdot\mathbf{u}\psi(\mathbf{x})d^3x, \tag{5b}$$

$$H_S=\frac{\hbar^2}{2m_3}\int d^2S\frac{\partial\psi^\dagger}{\partial z}u_z\frac{\partial\psi}{\partial z}, \tag{5c}$$

in which $\psi(x)$ is the electron annihilation operator. We show later that the effect of H_S can be neglected. We have also introduced n for the electron density, $N(0)$ for the electron density of states at the Fermi level, and m_3 the mass of the electron for motion in the z direction. This mass is often an order of magnitude less than the bare mass of the electron for surface levels of interest, which are associated with cylindrical portions of the Fermi surface.

We next specialize in the case of magnetic surface levels, in which the interesting electrons are confined to the surface region by a magnetic field in the y direction. Electric-field-induced levels can be treated analogously.

The zeroth-order Hamiltonian is therefore taken as[4]

$$H_0=\int\psi^\dagger\left(-\frac{\hbar^2}{2m_3}\frac{\partial^2}{\partial z^2}+\frac{eV_xHz}{c}+\epsilon(\mathbf{p})\right)\psi d^3x+\sum\hbar\omega_q a_{\mathbf{q}\lambda}{}^\dagger a_{\mathbf{q}\lambda}, \tag{6}$$

in which the Lorentz force has given rise to a potential which traps the electrons to the surface. The electronic eigenstates of (6) are

$$\psi_{n\mathbf{p}}=\phi_n(z)e^{i\mathbf{p}\cdot\mathbf{x}}/S^{1/2}, \tag{7}$$

where $\mathbf{p}$ is a vector parallel to the surface and ϕ_n is

$$\phi_n(z)=\alpha^{1/2}\,\mathrm{Ai}(\alpha z-a_n)/\mathrm{Ai}'(-a_n). \tag{8}$$

The wave number α in (8) is $\alpha=(2eHK/\hbar c)^{1/3}$ with $K=m_3V_x/\hbar$ standing for the Fermi-surface radius of curvature. The Airy function has been denoted Ai and its derivative Ai'. The zero of the function is at $a_n\approx[\frac{3}{2}\pi(n-\frac{1}{4})]^{2/3}$. The energies of states (7) are given by

$$E_{n,\mathbf{p}}=\epsilon(\mathbf{p})+E_n,$$

where

$$E_n=\hbar^2\alpha^2a_n/2m_3.$$

IV. LIFETIME OF ELECTRONIC STATES DEFORMATION CONTRIBUTION

We wish to discuss the lifetime of a state (7) against emission or absorption of a surface phonon coupled to it by means of H_D. A detailed calculation of this requires the solution of an integral equation, as the lifetime entering the conductivity can be quite different from the ordinary lifetime. Furthermore, the lifetime depends on the energy by which the electron exceeds the Fermi energy, and the number of phonons present. Since we shall be primarily interested in the temperature dependence of the lifetime and we shall eschew anything more than an estimate of the order of the magnitude of the lifetime, it will suffice to calculate the scattering rate of an electron at the Fermi surface due to the absorption of thermal surface phonons. The temperature dependence of this process is the same as that of an electron at excitation energy kT which can both emit and absorb phonons. For the moment we ignore the transport effects.

It is only sensible to consider the case of relatively low temperatures much below the Debye temperature, so that only rather long-wavelength thermal Rayleigh waves are present. Since the velocity $c_r\sim1.5\times10^5$ cm/sec is typical, one has for the typical wave number q_T of the Rayleigh wave at temperature T,

$$q_T=kT/\hbar c_r\sim10^6\,T(^\circ\mathrm{K})\ (\mathrm{cm}^{-1}).$$

The penetration of the compressional components of the Rayleigh wave is governed by the magnitude p, and so is very nearly the inverse of q_T. The shear components penetrate about three times farther.

At a temperature T_1 such that

$$q_{T_1}a_n/\alpha=1,$$

the Rayleigh wave just matches the penetration of the electron. Near this temperature the problem is complicated, so that we consider first the limiting case $T<T_1$. Under this condition H_D cannot cause a transition out of the state n to another state m, but can cause a transition from the initial state $\mathbf{p}$ to another $\mathbf{p}+\mathbf{q}$.

According to the Golden rule, the width of the state will be

$$\Gamma=\frac{2\pi}{\hbar}\sum_f|(\psi_fH_D\psi_i)|^2\delta(E_f-E_i),$$

which becomes, upon specializing to the case at hand,

$$\Gamma=\frac{2\pi}{\hbar}\int\frac{d^2q}{(2\pi)^2}\left(C\frac{q}{2\rho\omega_q/\hbar}\frac{n^2}{N(0)^2}\frac{c_r^2}{c_l^2}\right)\times N_qq^2\delta[\epsilon(\mathbf{p})+\hbar\omega_q-\epsilon(\mathbf{p}+\mathbf{q})]. \tag{9}$$

In (9) we have put $N_q=1/(e^{\hbar\omega_q/kT}-1)$ and $A^2=C^2/qS$. The latter has the explicit form

$$\frac{1}{C^2}=(1-\delta)^{1/2}\left(\frac{1-\frac{1}{2}\lambda}{1-\lambda}+\frac{1-\frac{1}{2}\delta}{1-\delta}-\frac{2}{1-\frac{1}{2}\lambda}\right),$$

where $\lambda=c_r^2/c_l^2$ and $\delta=c_r^2/c_l^2$. C is generally about unity. The factor c_r^2/c_l^2 in (9) arises because the dilation couples only to the compressional components of the displacement. By analogy with results for bulk electron-phonon coupling, inclusion of the shear coupling would lead to the same general form for the result. Note that although the density of states of the surface phonons is two-dimensional, the extra factor of q in the normalization ensures that the mean-square displacements remain finite, although they are, of course, somewhat larger than in the three-dimensional case.

It is now easy to perform the angular integration and obtain

$$\Gamma=C_1(c_r^2/c_l^2)(\bar{c}^4/c_r^4)\Gamma_b, \tag{10}$$

where C_1 is a constant of order unity and $\bar{c}$ is the mean phonon velocity occurring in Γ_b, the width due to bulk phonon emission. The temperature dependence of Γ_b is T^3. Thus, on the basis of this analysis, a T^3 law is expected to hold for $T<T_1$, and the surface-wave contribution is expected actually to exceed the bulk contribution.

Unfortunately, the temperature T_1 is rather low. Since $\alpha\sim10^5$ $(H$ gauss$)^{1/3}$, we have $T_1\sim10^{-1}$ °K. (At present, only rather low magnetic fields of some gauss are suitable for the observation of magnetic surface levels.) This part of the temperature range will be very difficult experimentally, therefore.

Actually, since what is measured experimentally is a surface conductivity, there are transport corrections to this result. This is especially indicated since the electron is scattered into another state of very similar properties to the first.

An analysis which we shall not provide here shows that in this case the correct lifetime should go as T^5, just as for the bulk conductivity in the case of bulk phonon scattering, and that there should be an additional two powers of $\bar{c}/c_r$ as compared with the bulk result. We shall not dwell further on this point, since the prediction is somewhat academic in view of the low temperature required for its validity.

At temperatures $T>T_1$ the dominant contribution comes from Rayleigh waves whose penetration is less than that of the surface state in question. In this case the width becomes

$$\Gamma=\frac{2\pi}{\hbar}D\int\frac{d^2q}{(2\pi)^2}\sum_m|(\phi_m e^{-pz}\phi_n)|^2 \times q^2N_q\delta[\epsilon(\mathbf{p})+\hbar\omega_q+E_n-\epsilon(\mathbf{p}+\mathbf{q})-E_m], \quad (11)$$

where D stands for the bracket in (9). The dependence on the angle between p and q through the term $\mathbf{V}_F\cdot\mathbf{q}$ in the δ function is very important, and as usual one must have $\mathbf{V}_F\cdot\mathbf{q}\ll V_Fq$. [We make the approximation $\epsilon(\mathbf{p})-\epsilon(\mathbf{p}+\mathbf{q})=\mathbf{V}_F\cdot\mathbf{q}\hbar$.] The latter quantity is large compared with both $\hbar\omega_q$ and E_n-E_m. Hence the angular integration gives just $1/V_Fq$ and in particular is independent of E_m, thus allowing the sum over m to be performed by closure. As a result, we need the expression

$$(\phi_n e^{-2pz}\phi_n)=\tfrac{1}{4}\alpha^3/p(p^2+\alpha^2a_n), \quad (12)$$

which is valid only for $p>\alpha/a_n$. Calling $a=q/p$, we have

$$\Gamma=\frac{Da^3}{2\pi\hbar V_F}\int_0^\infty q^2dq\,\frac{\alpha^3}{q(q^2+\alpha^2a_na^2)}N_q. \quad (13)$$

Putting $x=\hbar c_rq/kT$, one finds

$$\Gamma=\frac{D(\alpha a)^3}{2\pi\hbar V_F}\int_0^\infty dx\,\frac{x}{x^2+\alpha^2a_na^2/q_T^2}\,\frac{1}{e^x-1}. \quad (14)$$

The value of the integral depends on the magnitude of q_T as compared with $\alpha(a_n)^{1/2}$, which is the wave number of the surface state at the surface. If $q_T\gg\alpha(a_n)^{1/2}$, then Γ depends linearly on temperature whereas in the opposite limit, a T^2 dependence is forecast. Admittedly unless a_n is quite large, there is at most a small region such that $\alpha/a_n<q_T<\alpha(a_n)^{1/2}$ for which the T^2 dependence is valid. Introducing T_2 by $q_{T_2}=\alpha(a_n)^{1/2}$, we then have for $T>T_2$,

$$\frac{\Gamma}{\Gamma_b}=C_2\frac{c_r^2}{c_l^2}\frac{\bar{c}^{-4}}{c_r^2}\frac{\alpha^3}{q_T^3}\frac{q_T}{\alpha(a_n)^{1/2}}, \quad (15)$$

where C_2 is a constant of order unity. This ratio is a few percent at helium temperatures. It can be enhanced by working at lower temperatures, but of course the absolute magnitude of the scattering rate decreases. It is to be noted that the surface-phonon scattering rate depends on the magnetic field, as the $\frac{2}{3}$ power in the linear region.

In estimating the contribution arising from the shear components of the surface phonons, several competing factors must be borne in mind. On the one hand, there is an enhancement arising from the slower transverse velocities. This tends to be offset by a weaker coupling to the electrons, since an actual change of shape of the Fermi surface is required. A favorable factor is that the important electrons are associated with the cylindrical portions of the Fermi surface which are more than likely to occur at zone boundaries where the coupling to shear modes is strongest. One should also note that the shear wave penetration is determined by $k=q\times(1-c_r^2/c_l^2)^{1/2}$ instead of by $p\sim q$ so that the characteristic temperatures T_1 and T_2 are increased by a factor of about 3 for the shear mode contribution.

In the regime $T>T_1$ it is possible to neglect the transport corrections, since transitions between states of many different quantum levels m are involved. The surface conductivity is sharply peaked at frequencies corresponding to the level spacing E_m-E_n so that once a transition is made out of the state E_n it is effectively lost as far as a contribution to the resonant transition is concerned.

V. SURFACE CORRUGATION SCATTERING

For completeness, we here estimate the effect of the corrugation of the surface induced by the passage of a Rayleigh wave. Restricting consideration to the case $q_T>\alpha$, we have, using H_S and the Golden rule,

$$S=\frac{2\pi}{\hbar}\left(\frac{\hbar^2}{2m_3}\right)^2\alpha^3\sum_m\alpha^3\int\frac{d^2q}{(2\pi)^2}|V|^2 \times N_q\delta[\epsilon(\mathbf{p})+\hbar\omega_q+E_n-\epsilon(\mathbf{p}+\mathbf{q})-E_m],$$

where we put

$$|V|^2=\frac{|u_{zq}(z=0)|^2}{2\rho\omega_q/\hbar}=\frac{q}{2\rho\omega_q/\hbar}\frac{(1-\delta)\lambda^2}{4(1-\frac{1}{2}\lambda)^2}C^2.$$

The sum over m is estimated by replacing it by an integral. Let $p_z=\alpha(a_m)^{1/2}$. Then

$$\Gamma_S\approx\frac{2\pi}{\hbar}\left(\frac{\hbar^2}{2m_3}\right)^2V^2\alpha^3\frac{2}{\pi}\int dp_z\,p_z^2\int\frac{d^2q}{(2\pi)^2} \times N_q\delta\left(\epsilon(\mathbf{p})+\omega_q+\epsilon_n-\epsilon(\mathbf{p}+\mathbf{q})-\frac{\hbar^2p_z^2}{2m_3}\right)$$
$$\approx\frac{2\pi}{\hbar}\frac{\hbar^2}{2m_3}\frac{\alpha^3V^2}{\pi}\int\frac{d^2q}{(2\pi)^2}(2Kq\cos\theta)^{1/2}N_q.$$

In the last equation, the integral is over the region $\cos\theta>0$. The resulting integrals may be performed to obtain

$$\Gamma_S\approx0.048\times\frac{2\pi}{\hbar}\frac{\hbar^2}{2m_3}\alpha^3V^2K^{1/2}q_T^{5/2}.$$

Thus we estimate

$$\frac{\Gamma_S}{\Gamma_b}=\frac{\bar{c}^4}{c_r^4}\frac{1}{(q_T)^{1/2}}\frac{\alpha^3}{K^{5/2}}.$$

Since $K\sim10^7$ and $\alpha\sim10^5$ cm^{-1}, Γ_S is negligible. The smallness of this result is primarily due to the smallness

of the temperature-dependent part of the mean-square surface displacements from planarity, at the temperatures in question. The total zero-point motion of the surface is much larger, but this gives rise only to effective-mass shifts, etc., and not to lifetime effects. Not until a state of surface roughness is reached with displacements comparable with lattice constants, and momentum transfers to the scattered electrons comparable with the Fermi momentum, can surface roughness be effective in reducing the electron lifetime. This, to say the least, is readily achieved by less-than-perfect surface preparation.

VI. SUMMARY

We have estimated that one component of the electron scattering rate for the case of magnetic surface levels will have the following temperature dependence. At exceedingly low temperatures it will go as T^5, there will be a transition region and then a T^2 law, another transition region, and finally a linear law. In practice, the two transition regions may overlap sufficiently so that no intermediate T^2 behavior may be discernible. This transition region is generally in the temperature range of a fraction of a degree, but perhaps could be pushed up to the range of 1° by judicious choice of material. Experimentally, the main result is that of the linear behavior, together with the dependence of the magnetic field to the $\frac{2}{3}$ power. We do not minimize the difficulty involved in being able to analyze the experimental data carefully enough to extract this dependence.[4] However, we think the result novel enough that it would be of interest to find it in experiment.

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Phonon Frequencies of Alkali Metals

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Phonon frequencies of alkali metals are calculated using the single orthogonalized-plane-wave electron-ion matrix element and the dielectric functions due to Singwi *et al.* and to Geldart and Vosko. We have calculated the bare-ion potential by the Hartree-Fock-Slater method, where the Slater exchange potential is replaced by a modified Kohn-Sham exchange potential which approximates correlation effects according to the simple prescription of Robinson *et al.* The calculated phonon frequencies of Li, Na, K, and Rb are in good agreement with the neutron spectroscopy measurements.

I. INTRODUCTION

THE study of the lattice dynamics of metals may, in effect, be reduced to the investigation of the bare electron-ion interaction and the polarization function of the conduction electrons. Vosko *et al.*[1] gave a formulation for the electron-ion matrix element (EIME) using the single–orthogonalized-plane-wave (OPW) function for the wave function of the conduction electrons. They used this EIME to calculate the phonon frequencies of the simple metals Na, Al, and Pb. Taylor *et al.*[2] find that the single-OPW method gives a fair representation of the EIME for Na using the Prokofjew potential as the bare-ion potential. The single-OPW scheme is therefore justified for a simple metal like sodium, where the single-OPW is a good representation of the wave function for the conduction electrons in the metal under consideration.

In Sec. II, we discuss a method for constructing the crystal potential. To introduce the notation and to provide a base for the discussion of results, we have given an abbreviated résumé of the single-OPW EIME. The method for calculating the electronic part of the dynamical matrix and the results for phonon frequencies of Li, Na, K, Rb, and Cs are presented in Sec. III. The results are discussed in Sec. IV.

II. THEORY

For simple metals which possess a primitive unit cell, an element of the dynamical matrix $D_{xy}(\mathbf{q})$ for the phonon wave vector $\mathbf{q}$ is usually written as the sum of three terms:

$$D_{xy}(\mathbf{q})=D_{xy}{}^{(C)}(\mathbf{q})+D_{xy}{}^{(R)}(\mathbf{q})+D_{xy}{}^{(E)}(\mathbf{q}). \quad (1)$$

$D_{xy}{}^{(C)}(\mathbf{q})$ arises from the direct electrostatic interaction between ions, $D_{xy}{}^{(R)}(\mathbf{q})$ originates from the exchange overlap contribution of ion cores, and $D_{xy}{}^{(E)}(\mathbf{q})$ stems from the effective electron-ion interaction. $D_{xy}{}^{(C)}(\mathbf{q})$ is evaluated by Ewald's method.[3,4] Vosko[5] argues that

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