

Supersymmetry Across Nanoscale Heterojunction

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Abstract

We argue that supersymmetric transformation could be applied across the heterojunction formed by joining of two mixed semiconductors. A general framework is described by specifying the structure of ladder operators at the junction for making quantitative estimation of physical quantities. For a particular heterojunction device, we show that an exponential grading inside a nanoscale doped layer is amenable to exact analytical treatment for a class of potentials distorted by the junctions through the solutions of transformed Morse-Type potentials.

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To have a proper grasp of designing any semiconductor device that relies on a heterojunction, a complete understanding of the transport phenomena at interface is important [1]. Positive and negative carriers moving across a junction [2, 3] face an abrupt jump in potential due to the periodicity defects in crystal lattice at interface and varying electrical and optical properties of different materials bounding the heterojunction. Different values of the position-dependent conduction-band energy on the two sides separated by a junction results in a δ -like singularity at the interface [4] producing either a very deep, narrow well or a very high but a thin barrier that depends on the position of the junction. In these situations it is worth considering the transformed potential which in a supersymmetric context shares almost the same bound spectra but are free from such a singularity. A general version of supersymmetric transformation (see the monograph [5] for an up-to-date survey) allows to construct a hierarchy of potential chain which, in physical purpose, is useful to remove or embed arbitrary number of bound states. Since the position of a bound state is related to the pole-structure of the S matrix, its artificial designing can be utilized to improve the mobility of the carriers and thus having a desired output at the acceptor diode. A study of the spectral properties of the induced intertwined potentials across the heterojunction is thus of immense physical importance.

In actual microscopic description of the motion of electrons (or holes with $e \rightarrow -e$) across a semiconductor junction, it is known [6] that the supersymmetric structure of the underlying Dirac Hamiltonian describes unpaired ‘spin-up’ and ‘spin-down’ states in the conduction and valence band near Γ or L-point in the Brillouin zone that are localized at the junction. Note that the existing literature [7-11] does not apply to a practical semiconductor device where two graded mixed semiconductors are artificially glued (say $\text{Ga}_{1-x}\text{Al}_x\text{As}/\text{GaAs}$ heterojunction or Si-SiO_2 layer) since the role of ladder operators across the junction is unclear. Consequently the usual

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techniques of constructing the transformed potential fail in the effective-mass approximation which replaces actual wave function by envelope wave function. In this Report we show that the information about spectral properties of a given effective mass Hamiltonian having a δ -singularity at the heterojunction can be extracted from the supersymmetrically transformed Hamiltonian which is free from such a singularity. We apply our method for a particular $\text{Ga}_{1-x}\text{Al}_x\text{As}/\text{GaAs}$ semiconductor device to compute analytically local electron density based on inter subband energy levels and envelope wave functions obtained from a physically justifiable choice of grading function.

We start by considering two heterojunctions formed by an artificial joining of three different material layers (doped or pure). In the effective mass approximation the normalized envelope wave function of a single electron in the n -th subband moving along the normal to the surface of the material layer (xy -plane) obeys the Schrödinger equation [12] for the given Hamiltonian $H_0(z)$ in SI unit

$$H_0(z)\psi_n(z) \equiv \left(-\frac{d}{dz} \left[\frac{\hbar^2}{2m^*(z)} \frac{d}{dz} \right] + V_0(z) \right) \psi_n(z) = E_n \psi_n(z) \quad (1)$$

The effective mass m^* has a position-dependent variation $m_2(z)$ between two junctions at $z = a_1, a_2$ connecting continuously two known constant values m_1 and m_2 outside the junctions

$$m^*(z) = \sum_{j=1}^3 G_j m_j; \quad m_2(a_i) = m_i, \quad i = 1, 2. \quad (2)$$

In above equations G_j s are dimensionless Heaviside theta functions defined by the relations

$$G_1 = \Theta\left(\frac{a_1 - z}{a_0}\right), \quad G_3 = \Theta\left(\frac{z - a_2}{a_0}\right), \quad G_2 = 1 - (G_1 + G_3), \quad (3)$$

where $a_0 = 4\pi\epsilon_0\hbar^2/m_0e^2 = 0.0529$ nm is Bohr radius, ϵ_0 denoting permittivity of free space and m_0, e are free electron mass and charge. A general class of the potential $V_0(z)$ containing the δ -singularity at the junctions is

$$V_0(z) = \sum_{j=1}^3 G_j V_0^{(j)} - \frac{\hbar^2 m_2'}{a_0 m_2^2} \sum_{\ell=1}^2 \epsilon_\ell G_\ell G_{\ell+1} \delta\left(\epsilon_\ell \frac{z - a_\ell}{a_0}\right), \quad \left[m_2' \equiv \frac{dm_2}{dz}, \epsilon_\ell = (-1)^\ell \right]. \quad (4)$$

The actual form of the component potentials $V_0^{(j)}(z)$ will depend on chemical composition of materials in different regions and the applied electric and magnetic field.

We assume that inside each region (except for the junctions) the component Hamiltonians $H_0^{(j)} = -d/dz[(\hbar^2/2m_j)d/dz] + V_0^{(j)}$ possess formal solutions $\psi_E^{(j)}(z)$ for an arbitrary energy E . We shall prove that there exists transformed Hamiltonian $\tilde{H}_0(z)$ that shares the same spectra as H_0 but is free from δ -singularity. In other words using supersymmetric factorization we are going to construct a new potential of the form

$$\tilde{V}_0(z) = \sum_{j=1}^3 G_j \tilde{V}_0^{(j)}(z), \quad (5)$$

satisfying the above properties where $\tilde{V}_0^{(j)}(z)$ are non-singular. Note that the component Hamiltonians can always be projected in a factorized form

$$H_0^{(j)} = A_j A_j^\dagger - \mathcal{E}, \quad A_j = \frac{\hbar}{\sqrt{2m_j}} \frac{d}{dz} + W(z), \quad (6)$$

where the superpotential W is a continuous smooth function determined by the shape of the component potentials. Our aim is to factorize the given Hamiltonian H_0 in terms of the ladder operators which will act globally through the junction, i.e. $H_0 = AA^\dagger - \mathcal{E}$ (factorization energy \mathcal{E} is chosen to make spectra positive definite).

Since all junctions are quantum mechanically of equal preference it is reasonable to choose the form of the ladder operators at each junction as the average of the two adjacent component operators. This leads to the following representation of A :

$$A = \sum G_j A_j = \frac{\hbar}{\sqrt{2m^*}} \frac{d}{dz} + W(z) \quad (7)$$

It is straightforward to verify that the presence of theta functions in the ladder operators simulates δ -singularity in the given potential $V_0(z)$. It remains to show that the transformed Hamiltonian given by the factorized form

$$\tilde{H}_0(z) = A^\dagger A - \mathcal{E} \quad (8)$$

will not contain such a singularity. Clearly the wave function ψ of the given Hamiltonian (1) must be continuous in the entire region for otherwise Schrödinger equation (1) has to hold a stronger singularity than δ . Noting that the intertwining relation

$$H_0 A = A \tilde{H}_0 \quad (9)$$

relates ψ and $\tilde{\psi}$ as $\psi \propto A\tilde{\psi}$, we conclude that the action of A on $\tilde{\psi}$ must be continuous across junctions. Suppose that the wave functions $\tilde{\psi}$ of \tilde{H}_0 may be constructed as a superposition of component solutions $\tilde{\psi}_E^{(j)}$ where the average of two adjacent plain waves contributes equally at the junction. Using this construction and the representation (7) of the operator A we then arrive at the following matching conditions on $\tilde{\psi}$

$$\tilde{\psi}'(a_j + 0) = \tilde{\psi}'(a_j - 0) = \tilde{\psi}'(a_j). \quad (10)$$

where we have used the usual continuity condition for $\tilde{\psi}$. The smoothness of $\tilde{\psi}$ across junction indicates that transformed potential (5) is free from any singularity. This can be directly verified from the explicit expression of the transformed potential

$$\tilde{V}_0(z) = W^2 - \left(\frac{\hbar W}{\sqrt{2m^*}} \right)' - \mathcal{E}. \quad (11)$$

If one applies similar reasoning for $\tilde{\psi} \propto A^\dagger \psi$, a slope-discontinuity of ψ will appear at the junctions which is the signature of δ -singularity. This striking difference between two transformed Hamiltonians arises due to the non-commutativity of momentum and mass operators which we can exploit via supersymmetric transformation.

Equations (7),(10) and (11) constitute the central result of this Report establishing a way to apply supersymmetric transformation across heterojunction. The set of conditions in (10) yield a transcendental energy equation whose roots correspond to the allowed electronic energy levels for the given Hamiltonian except for the factorization energy \mathcal{E} . Finally we note that for practical application of above result the particular composition of material layers will guide the choice of the superpotential simulating the potential structure inside and outside the junction.

Let us consider a device made up of $\text{Ga}_{1-x}\text{Al}_x\text{As}/\text{GaAs}$ with the interface located at $z = 0$. The n-type $\text{Ga}_{1-x}\text{Al}_x$ layer is grown in two Regions I ($-z_h < z < -a_t$) and II ($-a_t < z < a_t$) and adjacent GaAs layer is grown in Region III ($a_t < z < z_t$) so that two heterojunctions are symmetrically placed about the origin. The potential $V_0(z)$ is generally formed from several contributions

$$V_0(z) = -e\phi(z) + V_h(z) + V_{\text{Im}}(z) + V_{\text{xc}}(z) \quad (12)$$

The electrostatic potential $\phi(z)$ satisfies Poisson's equation (SI unit)

$$\frac{d}{dz} \left[\epsilon_0 \kappa(z) \frac{d\phi}{dz} \right] = e n(z), \quad (13)$$

where $n(z) = \sum_n N_n \psi_n^2(z) - N_D(z) + N_{AC}(z)$ is the electron concentration in which $N_D(z), N_{AC}(z)$ denote the position-dependent donor and acceptor concentrations and $N_n(z)$ represents the number of electrons per unit of area (in units of cm^{-2}) in subband n : $N_n(z) = (m^*(z) k_B T / \pi \hbar^2) \ln[1 + \exp\{(E_F - E_n)/k_B T\}]$, E_F denoting Fermi energy. Since electrostatic potential has to be extrapolated between (1) and (13) in an iterated numeric procedure, we shall not consider it here. $V_{\text{Im}}(z)$ and $V_{\text{xc}}(z)$ are respectively image potential [arising due to the dielectric constant step $\kappa(z)$] and exchange-correlation potential due to electron-electron interaction in the channel. It is well-known that image potential cannot be incorporated in equation (1) as it involves singularity at the origin. This effect is usually realized into $V_{\text{xc}}(z)$ by adding an image term dependent on mutual coordinates of two interacting electrons in the population. However for $\kappa_b \approx \kappa_c$ [the subscripts b and c indicate the barrier ($\text{Ga}_{1-x}\text{Al}_x\text{As}$) and the channel (GaAs) sides of heterojunctions], image term could be ignored and exchange-correlation potential may be parameterized [13] as (in Hartree atomic unit of energy: $E_h = \hbar^2/m_0 a_0^2 \simeq 27.2$ eV)

$$V_{\text{xc}}(z) = -\frac{1}{2} K_{cr}^2(x) \frac{2\ell m^*(z)/m_0}{\kappa^2(z)} E_h, \quad (14)$$

where the dimensionless constant $K_{cr}(x)$ depends on the doping fraction $x = x(z)$ as

$$K_{cr}(x) = \sqrt{\frac{1 + 0.7734x \ln(1 + x^{-1})}{21\ell\pi x(4/9\pi)^{1/3}}} \quad (15)$$

For the analytical purpose, a suitable continuous functional form for $\kappa(z)$ is useful which connects two known values κ_b and κ_c of dielectric constant. A simple choice $\kappa(z) = \sqrt{2\ell m^*(z)/m_0}$ reduces $V_{\text{xc}}(z)$ to an x -dependent constant simulating doping-influenced shift in the energy scale where ℓ is a parameter adjusting with κ_b and κ_c . Usually in numerical process a linear interpolation is taken between the values in the barrier and channel side. We propose an exponential grading in the intermediate Region II to connect values in I and III. This is reasonable since in a sufficiently narrow thickness of layer II ($2a_t$ in unit of nm) it basically implies linear interpolation and add corrections with the increase of thickness. Hence following connection between known effective mass values $m_b = m_2(-a_t) = b m_0$ and $m_c = m_2(a_t) = c m_0$ on Region I and III will be adopted

$$m^*(z) = G_1 m_b + G_2 m_2 + G_3 m_c, \quad m_2 = m_0 \beta^2 e^{2\beta z/a_0} \quad (16)$$

where the dimensionless parameter β is related with mass-steps b, c on both sides and the grading constants are given by (3) with the replacement of $a_{1,2}$ by $\mp a_t$. The choice of the superpotential will be guided by the physical fact that Aluminium doping creates a barrier [14] for electrons to diffuse to Region I and so they are mobilized to acceptor site containing a GaAs quantum well. Thus the potential V_0 should have a barrier on left, a well at intermediate region and approaching a constant value on the right to make the electrons pass through. This situation can be realized by the following superpotential

$$W(z) = \frac{\hbar}{a_0 \sqrt{2m_0}} (\mathcal{A} - \mathcal{B} e^{-\beta z/a_0}). \quad (17)$$

Both parameters \mathcal{A} and \mathcal{B} are dimensionless. The latter parameter is free controlling the depth of well and the height of the barrier and the former is related with exchange-correlation term (14) through the definition $\mathcal{A} = \sqrt{K^2 - K_{cr}^2}$, $K \geq K_{cr}$. At critical value $K = K_{cr}$, the

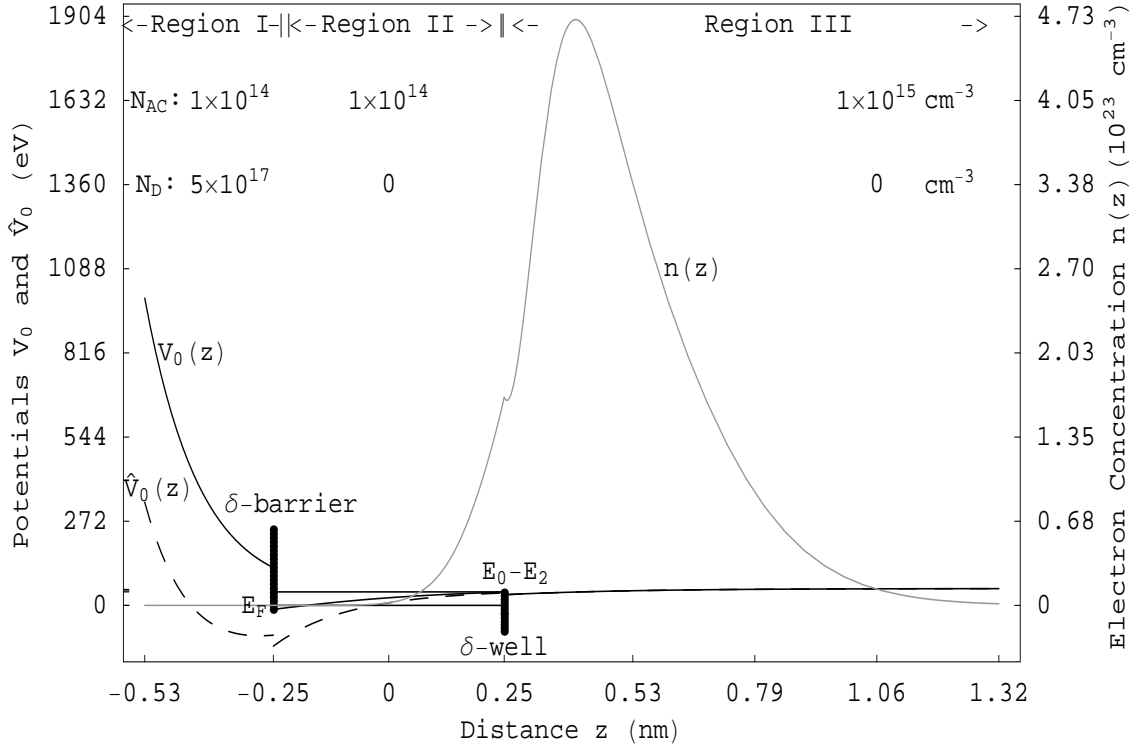


Figure 1: Original and transformed potentials with three levels $E_0 = 43.58$, $E_1 = 46.75$ and $E_2 = 51.67$ eV ($E_F = 35.9$ meV at 300 K) for the choice $\mathcal{A} = 2$, $\mathcal{B} = 1.1$, $\beta = 0.21$ and $a_t = 4.73$ which corresponds to 0.5nm intermediate layer thickness. Electron concentration is calculated using the data indicated in figure based on three wave functions obtained. Electrostatic term is not included.

doping-influence will be prominent, since it has very small values for $x = 0.3$ and 0.4 . Our strategy is to solve the transformed potential (5) according to the matching condition (10).

The add-on advantage of the model-choice (16) and (17) is that the component potentials $\widetilde{V}_0^{(j)}$ in three regions are of Morse type and so exact analytical solutions are available. The final expressions of unnormalized solutions for the transformed Hamiltonian are

$$\left. \begin{aligned} \tilde{\psi}_E^{(1)}(z) &= \exp[-\sqrt{b}\{\chi(z) + \sqrt{m_0\lambda z}\}]U(g_b, h_b, 2\sqrt{b\chi}) \\ \tilde{\psi}_E^{(2)}(z) &= \exp[\frac{\mathcal{B}\beta z}{a_0} - y(z)][M(g_2, h_2, 2y(z) + \varrho U(g_2, h_2, 2y(z))) \\ \tilde{\psi}_E^{(3)}(z) &= \exp[-\sqrt{c}\{\chi(z) + \sqrt{m_0\lambda z}\}]M(g_c, h_c, 2\sqrt{c\chi}) \end{aligned} \right\} \quad (18)$$

where $\chi(z) = \mathcal{B}e^{-\beta z/a_0}/\beta$, $y(z) = a_0\lambda\sqrt{m_0}e^{\beta z/a_0}$, $\lambda(E) = \sqrt{[\mathcal{A}^2/m_0a_0^2 - 2(E + \mathcal{E})/\hbar^2]}$ and $U(g, h, \xi)$, $M(g, h, \xi)$ are two linearly independent solutions [15] of confluent hypergeometric equations

$$\xi \frac{d^2w}{d\xi^2} + (h - \xi) \frac{dw}{d\xi} - gw = 0 \quad (19)$$

with the arguments $g_j = \sqrt{j(a_0\sqrt{m_0\lambda} - \mathcal{A})}/\beta$, $h_j = 1 + 2a_0\lambda\sqrt{m_j}/\beta$; $j = b, c$ and $g_2 = (2\mathcal{B} - 1)(\lambda - \mathcal{A})/2\lambda$, $h_2 = 2\mathcal{B} - 1$. The coefficient ϱ in the second equation of (18) is evaluated at solutions

of energy equation. The normalized envelope wave function of original Hamiltonian (1) for n -th subband $E_n(> 0)$ is

$$\psi_n(z) = \mathcal{N}_n(A\tilde{\psi}_{n+1}(z)), \quad \tilde{\psi}_n(z) = \sum_{j=1}^3 G_j \tilde{\psi}_{E_n}^{(j)}(z). \quad (20)$$

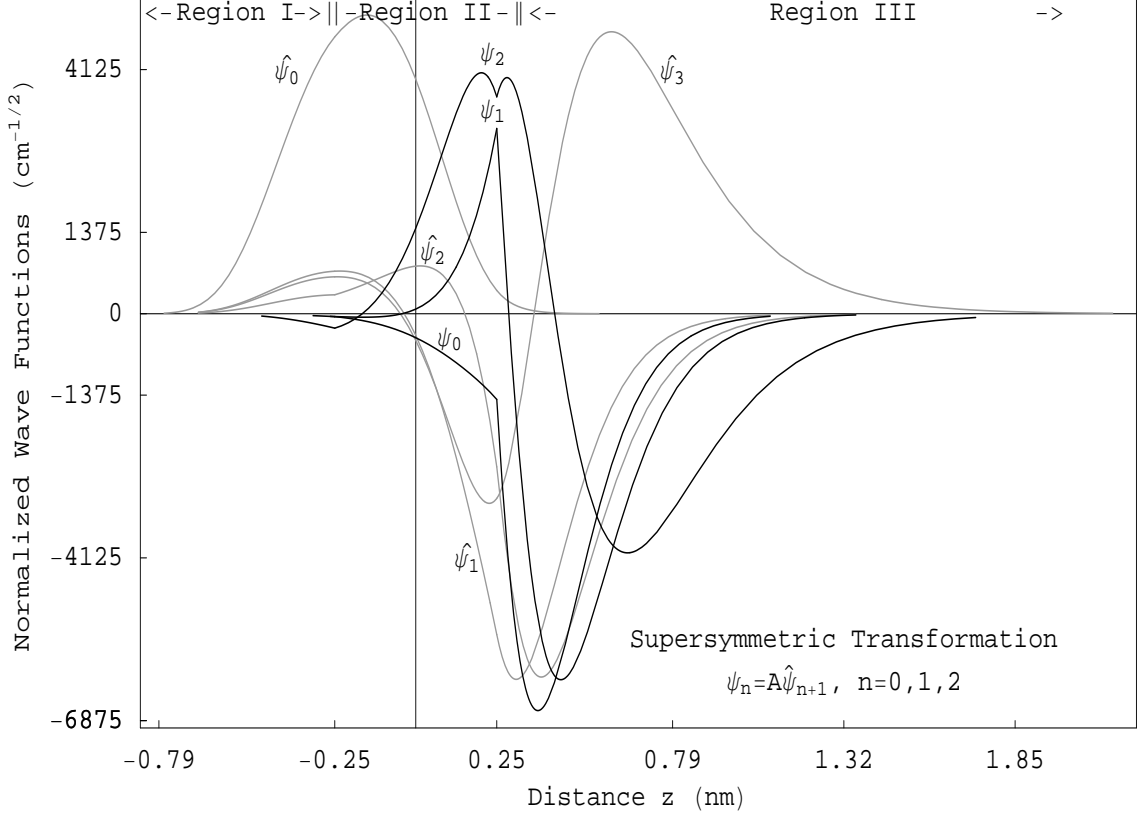


Figure 2: Envelope wave functions for the original and transformed potentials. Wave function for given potential is obtained by applying ladder operator A which suppresses one node. Electrostatic term is not included.

The energy equation is solved, using Mathematica, for representative values: $\mathcal{A} = 2$, $\mathcal{B} = 1.1$ and $\beta = 0.21$ with the intermediate layer thickness 0.5nm . Fig 1 shows the given potential (solid line) with δ -singularity and transformed potential (dashed line) with δ -singularity removed having four levels with zero energy ground state. Thus we choose $\mathcal{E} = 0$ and the three levels for given potential are shown. The levels are very close ($E_{10} = 3.17, E_{21} = 4.92$ eV) and lie at the bottom of the well above the Fermi energy $E_F = 35.9$ meV at 300K. Electron concentration (grey curve) is shown at 300K by choosing smooth continuous functional form around small intervals containing two junctions. Fig 2 shows the effect of supersymmetric transformations on wave functions $\tilde{\psi}_{n+1}, n = 0, 1, 2$ (Grey curves) which suppress one node to recover original wave functions ψ_n , as is expected. Higher levels for transformed potential violate oscillation theorem as δ -singularities resist creation of node near junctions. Interestingly original wave functions perfectly follow oscillation theorem leaving a sharp non-smoothness at the junction near channel side. Hence transformed Hamiltonian, which is free from δ -singularity, digests its effects and makes the original solutions physically acceptable.

To conclude, we have provided a method to bypass the essential δ -singularity in the effective-mass potential at the heterojunction using supersymmetric transformation. Note that the method is initiated from the observation that although original potential is invariably affected by δ -singularity at the heterojunction, its supersymmetric partner escapes such a singularity. We emphasize that this observation was unnoticed in the literature. Further, in spite of extensive works [7-11] regarding application of supersymmetry in position-dependent mass problems, no prescription existed to tackle the presence of heterojunction [2, 3] in semiconductor. This gap is filled in the present communication. Finally, for a particular $\text{Ga}_{1-x}\text{Al}_x\text{As}/\text{GaAs}$ device we have provided an exact analytical treatment based on a model grading function connecting values of band parameters across the junction. The choice of exponential grading function is subtle for exact analytical solution as it leads to a mapping in a constant-mass scenario to a known Morse potential in Region I and III which are joined by a distorted Morse-Type potential in the intermediate Region II.

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