

Density of states of a two-dimensional electron gas in low-dimensional diluted magnetic semiconductor

Mehdi M. Mahmudov, Ragib Y. Damirov*

Department of Solid State Physics, Baku State University, Baku, Azerbaijan

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Abstract

The density of states of a two-dimensional electron gas in low-dimensional diluted magnetic semiconductor is studied analytically. A single-particle Hamiltonian incorporating effective-mass kinetic energy, Landau quantization, ordinary Zeeman coupling, and the mean-field exchange interaction between conduction-band electrons and localized Mn ions is constructed, and a general form the density of states expression is obtained. The exchange term is evaluated via the Brillouin function, making the spin splitting strongly dependent on both temperature and Mn concentration x . Unlike non-magnetic two-dimensional systems, the density of states profile here is simultaneously tunable through three independent parameters magnetic field B , temperature T , and Mn concentration x a flexibility that makes diluted magnetic semiconductor superlattice particularly attractive for spintronics applications requiring a field-tunable, spin-resolved electronic structure.

Keywords: diluted magnetic semiconductor, superlattice, two-dimensional electron gas, density of states, Landau levels, exchange interaction, Zeeman splitting.

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1. Introduction

Diluted magnetic semiconductors (DMS) are alloys in which a fraction of the host cation sites is randomly substituted by magnetic transition-metal ions, most frequently Mn^{2+} . The resulting materials combine the band-structure tunability of

*Corresponding author – Tel.: (+994) 77 766 60 37

e-mail address: ragibdamirov@bsu.edu.az; ORCID ID: 0009-0008-8712-1310

conventional semiconductors with the magnetic properties conferred by the localized d-electrons of the impurity ions. This combination has attracted sustained interest because it enables the simultaneous manipulation of carrier charge and spin, which is the central objective of spintronics [1, 2]. The physical mechanism that sets DMS apart from both pure semiconductors and conventional magnetic materials is the $sp-d$ exchange interaction: the strong coupling between the spin of a band carrier and the localized spin of a neighboring Mn^{2+} ion ($S = 5/2$). This coupling produces a pronounced enhancement of spin splitting, strong magneto-optical activity, and a highly temperature-sensitive effective g-factor [3, 4].

When DMS materials are grown in the form of superlattices or quantum-well structures, quantum confinement adds a further degree of control: the dimensionality of the system is reduced, and the interplay between confinement, magnetic field, and exchange interaction gives rise to electronic properties with no counterpart in bulk DMS [5, 6]. A central quantity for characterizing any low-dimensional electron system is the density of states (DOS) function $g(\varepsilon)$. The DOS specifies how many single-particle quantum states are available per unit energy interval and thereby determines the thermodynamic response—chemical potential, heat capacity, entropy, magnetization—as well as kinetic coefficients such as electrical conductivity, thermoelectric power, and Hall coefficient [7, 8]. In two-dimensional systems the DOS takes the well-known staircase form in zero field; the application of a magnetic field converts this into a sequence of sharp peaks associated with Landau levels [9]. In DMS superlattices, spin splitting due to both the Zeeman effect and the exchange interaction further resolves each Landau peak into spin-polarized sub-peaks whose energy separation is strongly temperature- and concentration-dependent [10, 11]. Despite the extensive literature on DMS physics, a treatment that integrates Landau quantization, Zeeman splitting, Brillouin-function-mediated exchange, and Lorentzian level broadening into a single analytical framework for the DOS of a two-dimensional electron gas in a Mn-doped superlattice remains valuable.

2. Energy Spectrum and Wave Functions of Diluted Magnetic Semiconductor Superlattice

The single-particle Hamiltonian for an electron in a diluted semiconductor superlattice subject to a magnetic field \mathbf{B} directed along the z-axis is written as:

$$H = H_0 + H_B + H_C + H_{ex}. \quad (1)$$

H_0 is the kinetic energy operator in the effective-mass approximation, which accounts for the periodic crystal potential implicitly through the band effective mass. H_B incorporates both the orbital effect of the magnetic field (Landau quantization) and the ordinary spin Zeeman term proportional to the free-electron g-factor. H_C represents Coulomb interactions between carriers and between carriers and charged

impurities, treated here at the mean-field (Hartree) level. H_{ex} is the exchange Hamiltonian [12, 13]. The exchange Hamiltonian is cast in the Heisenberg form:

$$H_{ex} = - \sum J(\vec{r} - \vec{R}_n) S_n \sigma, \quad (2)$$

where $J(\vec{r} - \vec{R}_n)$ is the exchange integral associated with the n th Mn ion located at \vec{R}_n , S_n is the spin 5/2 operator of that ion, and σ is the electron spin operator. Within the mean-field approximation, the thermodynamic averages of the Mn spin operators replace their quantum-mechanical counterparts. The exchange contribution to the single-particle energy then reduces to a spin-dependent shift governed by the thermally averaged z-component of the Mn spin. When the magnetic field is directed along z , then in H_{ex} , all manganese spin operators are replaced by their mean values, and for the conduction band [21]:

$$\langle \psi_c | H_{ex} | \psi_c \rangle = \begin{vmatrix} 3A & 0 \\ 0 & 3A \end{vmatrix} \quad (3)$$

Here

$$A = -\frac{1}{6} N_0 \alpha \langle |S_z| \rangle x, \quad (4)$$

where N_0 is the number of cells per unit volume, the modification of the band structure caused by the interaction will be described by a constant α equal to $\alpha = -\langle S|J|S \rangle / \Omega$, x – the molar concentration of the impurity. In the Schrödinger equation, in the effective mass approximation, the exchange potential mixes the orbital and spin degrees of freedom, which can lead to the scattering of electrons from one orbital state to another with a spin flip. The solution to the Schrödinger equation with Hamiltonian (1) taking into account (3) for the energy spectrum of diluted magnetic semiconductor superlattices in a strong magnetic field parallel to the axis directed perpendicular to z the layers, which quantizes the motion of the electron in the plane of the layer and removes the spin degeneracy for the energy spectrum, will have the form:

$$\varepsilon(N, \sigma, k_z) = (2N + 1)\mu_B + \varepsilon_0(1 - \cos a k_z) + g^* \sigma \mu_B B + 3AS. \quad (5)$$

Where $N = 1, 2, \dots$ are the Landau quantum numbers, k_z is the quasi-momentum component along the axis z , $\mu = (m_0/m_\perp)\mu_B$, m_0 is the mass of a free electron, m_\perp is the mass of the electron in the plane of the layer, ε_0 is the half-width of the conduction band in the direction k_z , a is the superlattice period in the direction z , g^* is the factor that is determined from the band structure, and the remaining symbols carry their standard meanings. It can be seen that each Landau level is distributed into two spin sublevels, and the magnitude of the distribution of the N th level is the same and equal to $\Delta\varepsilon = g^* \mu_B B$. Manganese ions with spin 5/2 are taken as

impurities, and then the energy spectrum (5) takes the form:

$$\varepsilon = (2N + 1)\mu B \pm \frac{1}{2}g\mu_B B \mp \frac{5}{2}\alpha x f(B, T) + \varepsilon_0(1 - \cos a k_z). \quad (6)$$

Since the z-component of the electron spin commutes with the full Hamiltonian, it is a conserved quantity and the wave function factorizes into an orbital part and a Pauli spinor:

$$\psi(\vec{r}) = \psi_{nk}(\vec{r})\chi_\sigma, \quad (7)$$

with $\chi_\uparrow = \begin{pmatrix} 1 \\ 0 \end{pmatrix}$ for $\sigma = +1/2$ and $\chi_\downarrow = \begin{pmatrix} 0 \\ 1 \end{pmatrix}$ for $\sigma = -1/2$ Choosing the Landau gauge $\mathbf{A} = (0, Bx, 0)$ and invoking translational symmetry along y and z :

$$\psi_{nk}(x, y, z) = \varphi_N(x) \frac{1}{\sqrt{L_y}} e^{ik_y y} \frac{1}{\sqrt{L_z}} e^{ik_z z}, \quad (8)$$

The x-equation is a shifted harmonic oscillator with cyclotron frequency $\omega_c = eB/m_\perp$ and guiding-center coordinate $x_0 = \hbar k_y / eB$ [16]:

$$\left[-\frac{\hbar^2}{2m_\perp} \frac{d^2}{dx^2} + \frac{1}{2}m_\perp \omega_c^2 (x - x_0)^2 \right] \varphi_N(x) = E_N^\perp \varphi_N(x), \quad (9)$$

The normalized eigenfunctions are expressed through the N th Hermite polynomial H_N :

$$\varphi_N(x) = \frac{1}{\sqrt{2^N N!} \sqrt{\pi} R} H_N \left(\frac{x - x_0}{R} \right) \exp \left[-\frac{(x - x_0)^2}{2R^2} \right], \quad (10)$$

The complete wave function of the Mn-doped superlattice system is therefore:

$$\begin{aligned} \psi_{N,k_y,k_z}(x, y, z) &= \\ &= \frac{1}{\sqrt{L_y L_z 2^N N!} \sqrt{\pi} R} H_N \left(\frac{x - k_y R^2}{R} \right) \exp \left[-\frac{(x - k_y R^2)^2}{2R^2} \right] e^{i(k_y y + k_z z)}. \end{aligned} \quad (11)$$

3. Density of States of Diluted Magnetic Semiconductor Superlattice

The DOS per unit volume is defined as the number of accessible single-particle states per unit energy. For the system under consideration, it takes the form [17]:

$$g(\varepsilon) = \sum_N \int \frac{dk_z}{2\pi} \delta(\varepsilon - \varepsilon_N(k_z)) \quad (12)$$

where

$$\varepsilon_N(k_z) = (2N + 1)\mu_B \pm \frac{1}{2}g\mu_B B \mp \frac{5}{2}\alpha x f(B, T).$$

The delta function in (12) is appropriate for an ideal system with perfectly sharp quantum levels. In practice, several physical mechanisms broaden the Landau levels: scattering from ionized *Mn* impurities, alloy disorder inherent in the random distribution of Mn on cation sites, interface roughness in the superlattice, and electron–phonon coupling. These effects are collectively parametrized by replacing the delta function with a Lorentzian of half-width Γ [18]:

$$\delta(\varepsilon - \varepsilon_N(k_z)) \rightarrow \frac{1}{\pi} \frac{\Gamma}{(\varepsilon - \varepsilon_N(k_z))^2 + \Gamma^2}. \quad (13)$$

In high-quality molecular beam epitaxy grown II–VI DMS samples, Γ typically lies in the range 1–10 meV. Evaluating the integral in (12) by the stationary-phase method at the points k_z^* satisfying $\varepsilon = \varepsilon_N(k_z^*)$ yields:

$$g(\varepsilon) = \sum_N \sum_{k_z} \frac{1}{2\pi} \frac{1}{\left| \frac{d\varepsilon_N(k_z)}{dk_z} \right|_{k_z=k_z^*}} \quad (14)$$

In real systems, mechanisms such as impurity scattering, phonon interactions, electron-electron interactions, and surface scattering cause broadening of the energy levels, which is characterized by the parameter Γ . The delta function is replaced by a Lorentzian, and as a result, the sharp steps of the ideal system are transformed into smooth transitions in the real system. For an analytical study of the density of state function from energy, a graphical dependence was constructed (Fig. 1) based on the following parameters: $\varepsilon_0 = 10$ meV, $a = 5$ nm, $g = 2$, $x = 0.05$, $\alpha = 0.22$ eV [1]. The oscillations observed in the blue curve in the energy range 0.6–2.0 eV reflect the fact that the Landau levels have not completely vanished and represent the signature of Landau level structure in the density of states (Fig. 1).

As a result of broadening, the Lorentzian curves of neighboring Landau levels overlap with one another, and the density of states never falls to zero, which accounts for the metallic conductivity of the system. In diluted magnetic semiconductors, the exchange interaction and the large effective g – factor give rise to giant Zeeman splitting, whereby each Landau level is resolved into two distinct spin sub-levels. At high energies ($\varepsilon > 2.6$ eV), the kinetic energy of the electrons greatly exceeds the cyclotron energy, the quantization conditions are no longer satisfied, and the system crosses over into quasi-classical behavior. Inserting the full dispersion relation into (14) and carrying out the algebra leads to the general expression for the DOS of the *Mn* – doped superlattice in a magnetic field:

$$g_B(\varepsilon) = \frac{1}{2(\pi R)^2 a \varepsilon_0} \sum_{N\sigma} \sin^{-1}(ak_z). \quad (15)$$

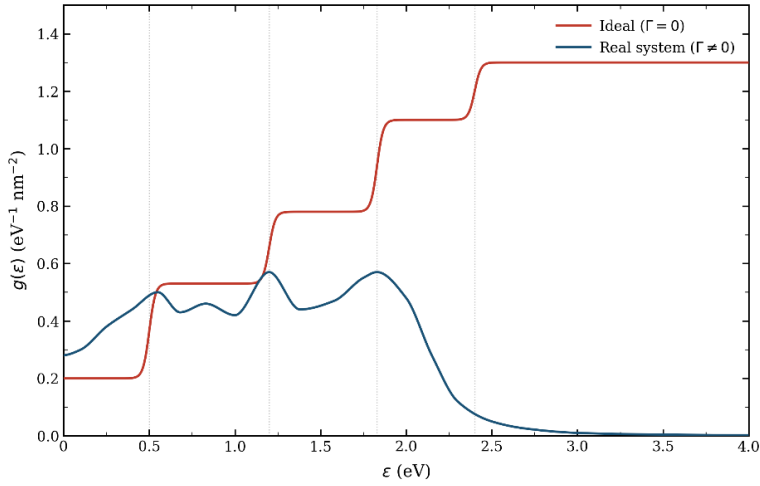


Fig. 1. Density of state dependence on energy $g(\epsilon)$.

Each Landau level is split by two additive mechanisms. The ordinary Zeeman effect separates spin-up and spin-down sub-levels by $\Delta\epsilon_{spin} = g^* \mu_B B$, a splitting that grows linearly with field. The exchange interaction introduces an additional temperature and concentration-dependent shift:

$$\epsilon_{ex} = \alpha x \langle S_z \rangle. \quad (16)$$

Because the exchange constant α is large in *Mn* –based II–VI compounds, the resulting effective g – factor satisfies $|g^*| \gg 1$ near the band edge at low temperatures, producing spin-resolved DOS peaks that are well separated even at moderate fields [19]. The net effect on the DOS near the Fermi level can be approximated as:

$$g(\epsilon, B) \approx g_0 \left(1 + \beta \frac{B}{B_0} \right), \quad (17)$$

where g_0 is the zero-field DOS, B_0 is a characteristic field set by the Landau level spacing, and β encodes the spin and exchange contributions. This approximate linear dependence holds in the smooth regime between singularities and breaks down at the peaks themselves.

4. Discussion

The DOS derived displays several features that are qualitatively distinct from those of both non-magnetic two-dimensional systems and bulk DMS materials, and it is worth examining these in detail. The most prominent feature is the set of Van Hove singularities appearing at the edges of each one-dimensional sub-band along k_z , as captured by the arcsine factor in equation (15). In an ideal system these sin-

gularities are logarithmically divergent; in a real sample they are resolved into Lorentzian peaks of finite height proportional to $1/\Gamma$. The number of observable peaks within a given energy window is determined by the ratio of the spin splitting to the Landau level spacing. When this ratio is small at high temperatures or low Mn concentrations the two spin sub-levels of each Landau level are nearly degenerate and the DOS appears as a single broadened peak per level, closely resembling the non-magnetic case [17]. As the temperature is lowered or the Mn concentration is increased, the Brillouin function grows and the exchange splitting pushes the two spin sub-levels apart, progressively resolving them into two distinct peaks per Landau level. This evolution from unresolved to resolved spin structure is a direct experimental signature of the $sp-d$ exchange mechanism and has been observed in magneto-optical and magneto-transport measurements on II–VI DMS quantum wells [10, 14]. The temperature sensitivity of the DOS is particularly noteworthy. Because $\langle S_z \rangle$ is governed by the Brillouin function rather than by a simple linear paramagnetic law, the temperature dependence of the spin splitting and hence of the DOS structure is highly non-linear. At temperatures above approximately 10K in typical $Cd_{1-x}Mn_xTe$ samples, the Brillouin function is in the dependence of linear and $\langle S_z \rangle \propto B/T$. Below this temperature it saturates and the splitting reaches its maximum value αx . In this saturated case the DOS is most strongly spin-resolved and the peaks are most sharply defined, providing the clearest experimental insight into on the exchange-enhanced Landau level structure [15, 20]. The role of the level-broadening parameter Γ deserves emphasis. When Γ is smaller than the spin splitting $\Delta\varepsilon_{ex}$, the two spin-resolved singularities per Landau level are individually resolvable. When Γ exceeds $\Delta\varepsilon_{ex}$, they merge into a single unresolved feature and the exchange splitting is effectively invisible in any DOS-derived observable. This condition places a practical lower bound on the sample quality specifically on the disorder level required to observe exchange effects in transport and thermodynamic measurements. High-quality molecular beam epitaxy with carefully controlled Mn incorporation is therefore essential for accessing the full structure predicted by equation (15) [18]. The concentration x of Mn ions provide an independent tuning parameter for the DOS. Increasing x at fixed temperature and field deepens the exchange correction ε_{ex} , widens the spin splitting, and shifts the Van Hove singularities to larger energy separations. It also increases disorder, however, since random Mn placement is an intrinsic source of alloy scattering that contributes to Γ . There is therefore an optimal value of concentration in which the exchange splitting is large enough to be resolved but the associated disorder broadening has not yet obscured it. This competition between exchange enhancement and disorder broadening is a recurring theme in DMS physics and governs the design of real devices based on these materials [1, 11].

5. Conclusions

A systematic theoretical treatment of the density of states for a two-dimensional electron gas in a low-dimensional diluted magnetic semiconductor superlattice has been developed. The analysis yields the following principal conclusions. The DOS acquires a highly structured spin-resolved structure of Van Hove singularities, one pair for each Landau level, arising from the one-dimensional dispersion of the superlattice along its growth axis. In the ideal limit these singularities are sharp; in realistic samples they are broadened into Lorentzian peaks of half-width Γ that is set by the combined disorder from alloy fluctuations, impurity scattering, and interface roughness. The spin splitting of each Landau-level peak has two physically distinct contributions: the ordinary Zeeman term, which scales linearly with the applied field, and the $sp-d$ exchange correction, which is mediated by the thermally averaged Mn spin $\langle Sz \rangle$ and therefore carries a strong, non-linear temperature dependence through the Brillouin function. The exchange contribution dominates at low temperatures and high Mn concentrations, where the effective g – factor far exceeds unity. The observability of the spin-resolved DOS structure depends on the competition between exchange splitting and level broadening. When the exchange splitting exceeds Γ , individual spin sub-peaks per Landau level are resolvable; when it does not, they merge into a single unresolved feature. Controlling this competition through sample quality and Mn concentration is the central materials challenge for accessing the full theoretical DOS structure experimentally. The Mn concentration x and the temperature T act as independent external controls for the DOS profile, supplementing the magnetic field B . This three-parameter tunability unavailable in non-magnetic two-dimensional systems is the defining practical advantage of DMS superlattices for device applications in which a field-tunable, spin-resolved electronic structure is desirable. The analytical expressions derived here for the DOS and its spin splitting provide the necessary theoretical foundation for subsequent calculation of thermodynamic observables-chemical potential, entropy, heat capacity, and magnetization as well as kinetic quantities including thermoelectric power and Hall conductivity of the electron gas in these systems.

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