

Comparison between approximate solution and exact solution for the bandedge energy of a magnetic semiconductor in the multiple scattering theory

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(Received November 25, 1998)

In the previous papers, we have assumed $\omega_b = \varepsilon_0 + \Sigma(\omega_b)$ to calculate the band bottom energy ω_b without further consideration. Here, ε_0 is the bottom energy of the undisturbed (model) band, and $\Sigma(\omega_b)$ is the self energy of an electron. In this work, we verify that above approximation gives rather good results within the discrepancy of 1%, comparing with the regroup results.

KEYWORDS: magnetic semiconductor, exchange interaction, coherent potential approximation (CPA)

§1. Introduction

In the previous papers,^{1,2)} we have successfully applied the single-site approximation for the s - f model in magnetic semiconductors. In the theory, the self energy of an electron, that is a complex which represents the effect of the disordered potential (or thermally fluctuating localized-spin) on the electron, is independent of its wave number k . In addition, at paramagnetic temperatures, the self energy is common for both orientations of electron's spin. Thus, the quasiparticle energy ω is given by $\omega = \varepsilon_k + \Sigma(\omega)$, where ε_k is the Bloch energy of an undisturbed electron, and $\Sigma(\omega)$ ($= \Sigma_{\uparrow}(\omega) = \Sigma_{\downarrow}(\omega)$) is the self energy. In addition, when calculating the lowest bandedge energy ω_b , it was assumed that

$$\omega_b = \varepsilon_0 + \Sigma(\omega_b), \quad (1)$$

with no further discussions on the validity. Here, ε_0 is the lowest bandedge energy of the model (undisturbed) band. Similar treatments were also done by Twolzydlo to investigate the behavior of the lowest bandedge energy of diluted magnetic semiconductors.³⁻⁵ However, the expression of Eq. (1) is not an exact one but only an approximate one.

The purpose of this work is to show the above approximation (or Eq. (1)) to be effective. For that sake, we calculate the bandedge energy of a magnetic semiconductor by two methods: the above-mentioned approximate solution and the exact solution. Comparing these results, we estimate the difference between approximate solution and exact solution.

§2. Basic Consideration

2.1 Coherent potential approximation for the s - f model

The s - f model is currently accepted as a basis for studying the conduction-electron states in ordinary magnetic semiconductors such as Eu-chalcogenides. In the s - f model, the Hamiltonian for an s electron interacting with f spins through the s - f exchange interaction is

$$H = \sum_{k,\mu} \varepsilon_k a_{k\mu}^\dagger a_{k\mu} - I \sum_{m,\mu,\nu} a_{m\mu}^\dagger \boldsymbol{\sigma} \cdot \mathbf{S}_m a_{m\nu} . \quad (2)$$

The total Hamiltonian, H_t , consists of H and H_f , where H_f represents the Heisenberg-type exchange interaction between f spins.

Applying the coherent potential approximation (CPA) for the s - f model at paramagnetic temperatures, we obtain the condition for Σ :^{1,6,7)}

$$\Sigma = F(IS + \Sigma)[I(S + 1) - \Sigma] , \quad (3)$$

with,

$$F(\omega) = \frac{1}{N} \sum_k \frac{1}{\omega - \varepsilon_k - \Sigma} . \quad (4)$$

In order to calculate $F(\omega)$, in this study, introducing the semicircular band with a half-bandwidth of Δ ,

$$\rho(\varepsilon) = \frac{2}{\pi\Delta} \sqrt{1 - \left(\frac{\varepsilon}{\Delta}\right)^2} , \quad (5)$$

as an undisturbed (model) density of states (i.e., for $IS = 0$), the summation over k in Eq. (4) is replaced by the integration of ε . Note $\omega_0 = -\Delta$.

2.2 Approximate solution of Eq. (1) for the bandedge energy

For $\omega = \omega_b$, putting Eq. (1) or $\omega_b = -\Delta + \Sigma$ into $F(\omega)$,

$$F(\omega_b)\Delta = \frac{2}{\pi} \int_{-\Delta}^{\Delta} d\varepsilon \sqrt{1 - \left(\frac{\varepsilon}{\Delta}\right)^2} \frac{1}{\omega_b - \varepsilon - \Sigma(\omega_b)} = -2. \quad (6)$$

Using the CPA condition Eq. (2), together with $F(\omega_b) = -2/\Delta$, we obtain two lower bandedge energies:

$$\frac{\omega_b}{\Delta} = -1 + \frac{\Sigma(\omega_b)}{\Delta} \quad (7)$$

$$= -1 + \frac{1}{2} \left\{ \left(\frac{I}{\Delta} + \frac{1}{2} \right) \pm \sqrt{\left(\frac{I}{\Delta} + \frac{1}{2} \right)^2 + 4 \left(\frac{IS}{\Delta} \right)^2 \left(1 + \frac{1}{S} \right)} \right\} \quad (8)$$

On the other hand, assuming the highest bandedge energy, $\omega_t = \Delta + \Sigma$ leads to $F(\omega_t)\Delta = +2$, instead of Eq. (6). Using the CPA condition Eq. (2), together with $F(\omega_t) = +2/\Delta$, we obtain two higher bandedge energies,

$$\frac{\omega_t}{\Delta} = 1 + \frac{\Sigma(\omega_t)}{\Delta} \quad (9)$$

$$= 1 + \frac{1}{2} \left\{ \left(\frac{I}{\Delta} - \frac{1}{2} \right) \pm \sqrt{\left(\frac{I}{\Delta} - \frac{1}{2} \right)^2 + 4 \left(\frac{IS}{\Delta} \right)^2 \left(1 + \frac{1}{S} \right)} \right\} \quad (10)$$

2.3 Exact solution for the bandedge energy ⁸⁾

For the semicircular model band, Eq. (5), we have

$$F(\omega)\Delta = \int_{-\Delta}^{\Delta} d\varepsilon \rho(\varepsilon) \frac{\Delta}{\omega - \varepsilon - \Sigma} = \frac{2}{\pi} \int_{-1}^1 dz \frac{\sqrt{1-z^2}}{L-z} = 2(L - \sqrt{L^2-1}) \quad (11)$$

where

$$L \equiv \frac{\omega - \Sigma}{\Delta}. \quad (12)$$

Next, using Eqs. (11) and (12), we define a new variable ξ , and a new function $f(\xi)$ by

$$\xi \equiv F^{-1} + \Sigma = \omega - \frac{\Delta^2}{4} F, \quad (13)$$

$$f(\xi) \equiv \frac{4}{\Delta^2} \xi + \left(\frac{S}{2S+1} \right) \frac{1}{\xi - E_a} + \left(\frac{S+1}{2S+1} \right) \frac{1}{\xi - E_p}, \quad (14)$$

where $E_p \equiv -IS$, $E_a \equiv I(S+1)$, and $F \equiv F(\omega)$. Now, the CPA condition Eq. (3) is rewritten as,

$$f(\xi) = \frac{4}{\Delta^2} \omega. \quad (15)$$

The CPA condition Eq. (15) is a cubic equation of ξ , so that the equation has three real roots or one real root and two complex conjugate roots. In the former case, $F(\omega)$ is real and hence the density of states vanishes at the energy ω . In the latter case, the density of states is nonvanishing at the energy ω . The real root is meaningless. When we draw the function $y = f(\xi)$ as a function of ξ , together with $y = 4\omega/\Delta^2$ in a figure, the intersections correspond to above roots. Thus, the band-edges correspond to the maximum or the minimum of $y = f(\xi)$. Consequently, the condition to determine ξ at which $f(\xi)$ takes the maximum or the minimum is,

$$\frac{d}{d\xi} f(\xi) = \frac{4}{\Delta^2} - \left(\frac{S}{2S+1} \right) \frac{1}{(\xi - E_a)^2} - \left(\frac{S+1}{2S+1} \right) \frac{1}{(\xi - E_p)^2} = 0. \quad (16)$$

Eq. (16) leads to the condition for bandedge energy,

$$\xi^4 + a\xi^3 + b\xi^2 + c\xi + d = 0, \quad (17)$$

with

$$a = -2I, \quad (18)$$

$$b = I^2 \{1 - 2S(S+1)\} - \frac{\Delta^2}{4}, \quad (19)$$

$$c = 2S(S+1)I^3 + \frac{\Delta^2 I}{2}, \quad (20)$$

$$d = I^4 S^2 (S+1)^2 - \frac{\Delta^2 I^2 \{S^3 + (S+1)^3\}}{4(2S+1)}. \quad (21)$$

For each root ξ of Eq. (17), bandedge energy ω_p is calculated using

$$\omega_p = \xi + \frac{\Delta^2}{4} \left[\left(\frac{S}{2S+1} \right) \frac{1}{\xi - E_a} + \left(\frac{S+1}{2S+1} \right) \frac{1}{\xi - E_p} \right]. \quad (22)$$

2.4 Exact condition for the band splitting^{7,8)}

When the curve of function $f(\xi)$ has a maximum and a minimum in the region of $-IS < \xi < +I(S+1)$, the band splitting happens. Thus, the condition for the band splitting is that the maximum accords the minimum. This means the maximum and the minimum happen at the changing point in the bending. The condition to decide the changing point in the bending, ξ , is,

$$\frac{d^2}{d\xi^2}f(\xi) = \left(\frac{2S}{2S+1}\right) \frac{1}{(\xi - E_a)^3} + \left(\frac{2(S+1)}{2S+1}\right) \frac{1}{(\xi - E_p)^3} = 0. \quad (23)$$

Eq. (23) leads to

$$\xi = \frac{S+1 - S\sqrt[3]{\frac{S}{S+1}}}{1 + \sqrt[3]{\frac{S}{S+1}}}. \quad (24)$$

The condition of bandsplitting is

$$\frac{d}{d\xi}f(\xi) = 0, \quad (25)$$

at the ξ given by Eq. (24). Eq. (24) leads the band splitting condition,

$$I = \frac{1}{2} \left[\frac{S^{\frac{1}{3}} + (S+1)^{\frac{1}{3}}}{2S+1} \right]^{\frac{3}{2}}. \quad (26)$$

§3. Result and Discussion

In Fig.1 we show the bandedge energies ω as a function of IS/Δ for $S = 1/2, 5/2, 7/2$ and classical spin $S = \infty$. The solid line represents the results for the exact solution given by Eqs. (17)-(22). The dashed line represents the results for the approximate solution given by Eqs. (8) and (10). The approximate solution for the top- and bottom energies of the band agree well the one of approximate solution in any value of S . It is verified that the difference in the energy of the band bottom between approximate solution and exact solution is within 1%. Thus, Eq. (1) is well applicable to investigate the band bottom energy. But, it should be noted that the approximate solution does not predict the band splitting condition.

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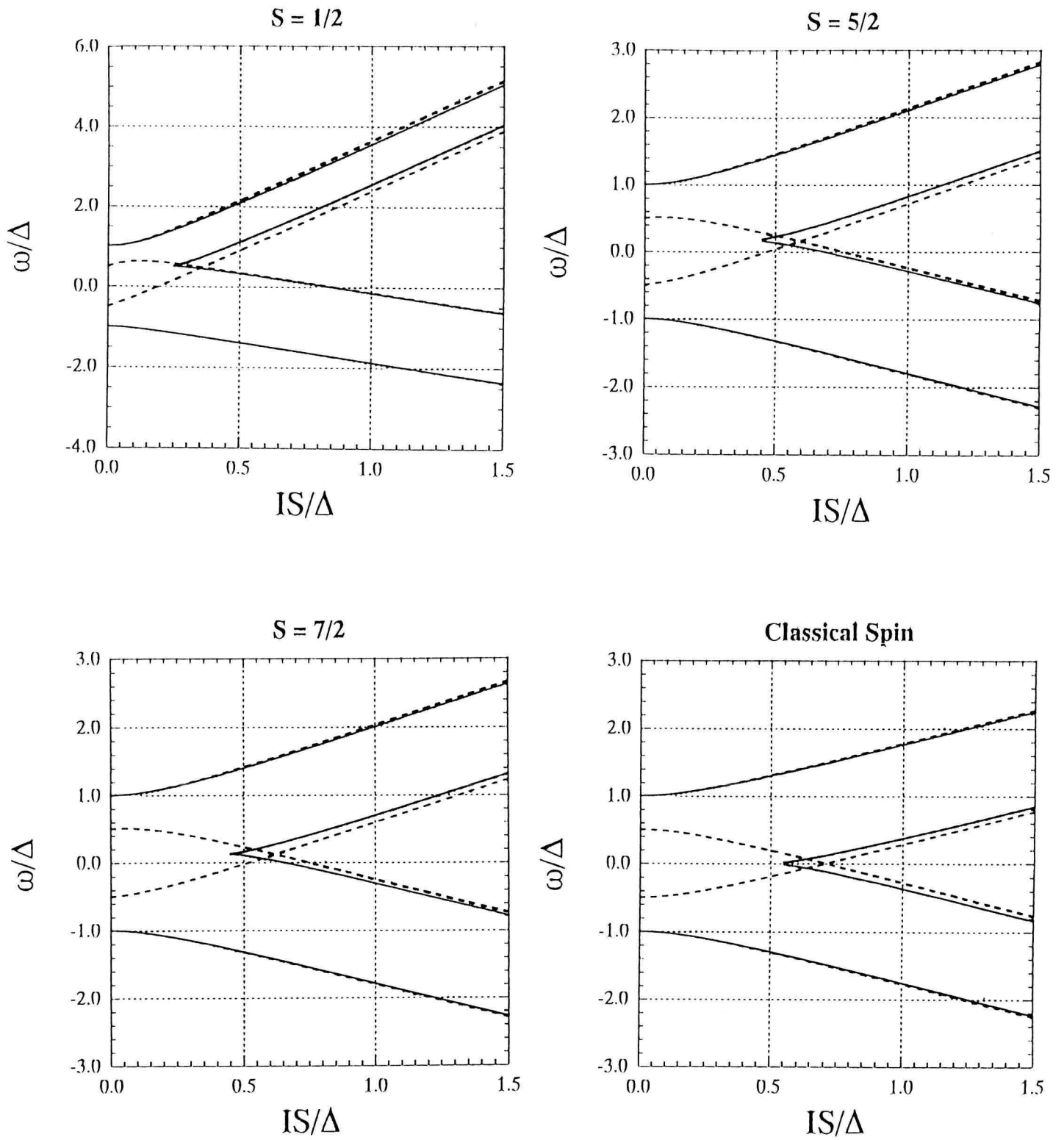


Fig. 1. Result for the exact solution (solid line) and the approximate solution (dashed line). (a) $S = 1/2$ (b) $S = 5/2$ (c) $S = 7/2$ (d) $S = \infty$