Exciton diamagnetic shift in semiconductor nanostructures

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A method is presented for calculating the diamagnetic coefficient of an exciton in a semiconductor nanostructure. The diamagnetic coefficient characterizes the response of a confined exciton to a weak magnetic field, and gives information about the roles of confinement and of the Coulomb interaction in determining the optical properties. A general formulation is presented for nanostructures of arbitrary size, shape, and dimensionality. We introduce a generalized gauge transformation that allows us to express the diamagnetic coefficient in terms of two characterizations of the size of an exciton, one involving confinement and the other involving the Coulomb interaction. Calculations of the diamagnetic coefficient are given for quantum well, wire, and dot geometries. [S0163-1829(98)00416-0]

I. INTRODUCTION

The optical properties of semiconductor nanostructures are of interest both because of their potential for application in optoelectronic devices and because of the insight they provide into the nature of confined electrons and holes. Excitons dominate the optical properties of these structures, typically producing sharp absorption and luminescence lines. In recent work, in particular, the properties of excitons are being studied to gain insight into confinement in quantum wires and dots.

Two factors are responsible for the properties of the exciton in a nanostructure. The first is confinement of the electron and the hole by the nanostructure. The second is the Coulomb interaction between the electron and the hole. Confinement can be controlled through the size and shape of the nanostructure as well as by the selection of structure and barrier materials to produce various band offsets. Confinement localizes the electron and hole, enhancing exciton binding energies and oscillator strengths. The Coulomb interaction is controlled by the static dielectric constant of the nanostructure material and produces exciton binding. Both factors significantly influence the energy and oscillator strength of a confined exciton.

External perturbation of a system, such as the application of an electric or magnetic field, can give valuable information about the exciton. An applied magnetic field has two effects on the spectroscopically observed energy levels. The first is the spin splitting of levels, which is linear in the applied field. The second is the diamagnetic shift, an increase in energy of both of the spin-split levels with magnetic field. The diamagnetic shift of an exciton in a quantum well has been treated by a number of authors.[1–8] It is our goal to extend this work to systems with lateral confinement.

In the case of a weak applied magnetic field, the energy increases quadratically with the applied field. We expect the energy to be quadratic in the magnetic field as long as the energy shifts are small compared to the exciton binding energy. This quadratic shift in energy of the exciton emission with an applied magnetic field gives information about the effects of confinement and of the Coulomb interaction in semiconductor nanostructures. The energy of the exciton can be written

$$E(B)=E_0+\gamma_1 B+\gamma_2 B^2+\cdots. \tag{1.1}$$

For a given direction of the applied magnetic field, the diamagnetic shift is characterized by a single number, the diamagnetic coefficient γ_2, which describes the low-field limit of the diamagnetic shift.

Exciton diamagnetic coefficients have come to be of considerable interest in the study of semiconductor nanostructures. This is in part because the diamagnetic coefficients are taken to be a measure of the effects of confinement,[9] and also because they are used to estimate exciton binding energies.[10,11] Nevertheless, to date there has not been a quantitative connection between the diamagnetic coefficients in these systems and the effects of confinement. It is part of the intention of the present work to establish this connection.

In this paper, we develop a variational technique to calculate the diamagnetic coefficient γ_2, and show that it is related to characterizations of the exciton size. These characterizations of exciton size can be seen to arise from the effects of confinement and electron-hole Coulomb interaction.

The Hamiltonian for a confined exciton in a magnetic field consists of a part independent of magnetic field, a part linear in magnetic field, and a part quadratic in magnetic field. If one were to use perturbation theory to calculate the diamagnetic coefficient with the zero-field states as the unperturbed states, one would need to use enough orders of perturbation to include all energy terms proportional to B^2. There are two such energy terms. One comes from the first-order contribution of the quadratic part of the Hamiltonian and the other comes from the second-order contribution of the linear part of the Hamiltonian. Each is dependent on the choice of gauge for the magnetic field, but together, they are gauge independent.[1] We present a generalized gauge transformation that is capable of eliminating the second-order contribution of the linear part of the Hamiltonian. Then, the diamagnetic coefficient is expressed as the expectation value of the coefficient of the quadratic part of the Hamiltonian.

In Sec. II we formulate a variational method to calculate the diamagnetic coefficient. In Sec. III we discuss the meaning of the four variational parameters used in the procedure and the reduction of the number of parameters necessary when there is symmetry in the confining potential. Section IV contains calculations of the diamagnetic coefficient for quantum well, wire, and dot structures and some conclusions.

II. EXCITON DIAMAGNETIC COEFFICIENT

A. General formulation

Within the effective-mass approximation, in the absence of a magnetic field, the Hamiltonian for an exciton in a confined structure is given by

$$H_0=\sum_{i=e,h}\sum_{\alpha=x,y,z}\frac{p_{i\alpha}^2}{2m_{i\alpha}}+V_e(\mathbf{r}_e)+V_h(\mathbf{r}_h)+V_c(|\mathbf{r}_e-\mathbf{r}_h|), \tag{2.1}$$

in which $p_{i\alpha}$ is the component of momentum for particle i (electron or hole) in direction α (x, y, or z), $m_{i\alpha}$ is the effective mass of particle i in direction α, $V_e(\mathbf{r}_e)$ is the potential energy of confinement for the electron, $V_h(\mathbf{r}_h)$ is the potential energy of confinement for the hole, and $V_c(|\mathbf{r}_e-\mathbf{r}_h|)$ is the Coulomb interaction between the electron and the hole. We use H_0 here to designate the Hamiltonian in the absence of a magnetic field. The Coulomb interaction between the electron and hole is

$$V_c(r)=-\frac{e^2}{\epsilon r}, \tag{2.2}$$

where $e=|e|$ is the hole charge, ϵ is the static dielectric constant, and $r=|\mathbf{r}_e-\mathbf{r}_h|$ is the relative electron-hole coordinate. We ignore electron and hole spin.

In the presence of a static, uniform magnetic field, the mechanical momenta $P_{i\alpha}$ are expressed in terms of the canonical momenta $p_{i\alpha}$ by

$$P_{i\alpha}=p_{i\alpha}-\frac{q_i}{c}A_\alpha(\mathbf{r}_i), \tag{2.3}$$

where $q_e=-e$, $q_h=e$, and $\mathbf{A}$ is the vector potential of the magnetic field. Then the Hamiltonian is

$$H=\sum_{i=e,h}\sum_{\alpha=x,y,z}\frac{P_{i\alpha}^2}{2m_{i\alpha}}+V_e(\mathbf{r}_e)+V_h(\mathbf{r}_h)+V_c(|\mathbf{r}_e-\mathbf{r}_h|). \tag{2.4}$$

We can in general write the exciton wave function in the presence of a magnetic field as

$$\Psi(\mathbf{r}_e,\mathbf{r}_h)=\chi(\mathbf{r}_e,\mathbf{r}_h)e^{-i\phi(\mathbf{r}_e,\mathbf{r}_h)}, \tag{2.5}$$

where χ and ϕ are real functions. We then have

$$\langle\Psi|H|\Psi\rangle=\langle\chi e^{-i\phi}|H|\chi e^{-i\phi}\rangle=\langle\chi|e^{i\phi}He^{-i\phi}|\chi\rangle =\langle\chi|H'|\chi\rangle, \tag{2.6}$$

where H' is defined as

$$H'=e^{i\phi}He^{-i\phi}. \tag{2.7}$$

The ground-state energy of the exciton in a given magnetic field is found by minimizing the expectation value of the Hamiltonian:

$$E(B)=\min_{\Psi}\frac{\langle\Psi|H|\Psi\rangle}{\langle\Psi|\Psi\rangle}=\min_{\chi,\phi}\frac{\langle\chi|H'|\chi\rangle}{\langle\chi|\chi\rangle}=\min_{\chi,\phi}\langle H'\rangle, \tag{2.8}$$

where we have introduced the shorthand notation for the expectation value of an operator A,

$$\langle A\rangle=\frac{\langle\chi|A|\chi\rangle}{\langle\chi|\chi\rangle}. \tag{2.9}$$

The functions χ and ϕ that minimize $\langle H'\rangle$ will vary with B. Evaluation of Eq. (2.7) with Eq. (2.4) gives

$$H'=\sum_{i=e,h}\sum_{\alpha=x,y,z}\frac{P'^2_{i\alpha}}{2m_{i\alpha}}+V_e(\mathbf{r}_e)+V_h(\mathbf{r}_h)+V_c(|\mathbf{r}_e-\mathbf{r}_h|) \tag{2.10}$$

with

$$P'_{i\alpha}=P_{i\alpha}-\hbar\frac{\partial\phi}{\partial x_{i\alpha}}=p_{i\alpha}-\frac{q_i}{c}A_\alpha(\mathbf{r}_i)-\hbar\frac{\partial\phi}{\partial x_{i\alpha}}. \tag{2.11}$$

Here we have performed a generalized gauge transformation. It is generalized in the sense that we have added the gradient of a scalar function of six spatial dimensions to the six-dimensional vector potential expressed as a function of electron and hole coordinates, rather than the usual three-dimensional vector potential whose curl gives the external magnetic field. We can now form the expectation value of H' with respect to χ. The expectation value of the term linear in $p_{i\alpha}$ vanishes because χ is real, and we have the result

$$\langle H'\rangle=\langle H_0\rangle+\sum_{i=e,h}\sum_{\alpha=x,y,z}\frac{1}{2m_{i\alpha}}\left\langle\left[\frac{q_i}{c}A_\alpha(\mathbf{r}_i)+\hbar\frac{\partial\phi}{\partial x_{i\alpha}}\right]^2\right\rangle. \tag{2.12}$$

We are interested in the expansion of the energy in powers of B as in Eq. (1.1). Hence, rather than minimizing the expectation value of the Hamiltonian at each value of B, we expand the expectation value of the Hamiltonian and minimize the coefficients in the expansion:

$$\langle H'\rangle=[\langle H'\rangle]_{B=0}+\left[\frac{d\langle H'\rangle}{dB}\right]_{B=0}B+\left[\frac{1}{2}\frac{d^2\langle H'\rangle}{dB^2}\right]_{B=0}B^2+\cdots. \tag{2.13}$$

We allow the functions ϕ and χ to vary with B by expanding ϕ in a series in B,

$$\phi(B)=\phi_0+\phi_1B+\phi_2B^2+\cdots, \tag{2.14}$$

and by allowing χ to be determined by a set of variational parameters α_i which we expand in powers of B,

$$\alpha_i(B)=\alpha_i^{(0)}+\alpha_i^{(1)}B+\alpha_i^{(2)}B^2+\cdots. \tag{2.15}$$

The coefficients of the powers of B in Eq. (2.13) can be consistently and independently minimized to give

$$E_0 = \min[\langle H' \rangle]_{B=0}, \tag{2.16}$$

$$\gamma_1 = \min\left[\frac{\partial \langle H' \rangle}{\partial B}\right]_{B=0},$$

$$\gamma_2 = \min\left[\frac{1}{2}\frac{\partial^2 \langle H' \rangle}{\partial B^2}\right]_{B=0},$$

where the minimizations are now with respect to $\alpha_i^{(n)}$ and ϕ_i. Details of this derivation are given in the Appendix. The result is

$$\gamma_2 = \min_{\phi_1} \sum_{i=e,h} \sum_{\alpha=x,y,z} \frac{1}{2m_{i\alpha}} \left\langle \left[\frac{q_i}{2c} a_\alpha(\mathbf{r}_i) + \hbar \frac{\partial \phi_1}{\partial x_{i\alpha}} \right]^2 \right\rangle, \tag{2.17}$$

where the expectation value is with respect to the exciton ground state at zero magnetic field. We have defined a vector field **a** such that $\mathbf{A} = (B/2)\mathbf{a}$. A further simplification results by defining $\overline{\phi} = (2\hbar c/e)\phi_1$. Then we have that the diamagnetic coefficient is given by

$$\gamma_2 = \min_{\overline{\phi}} \sum_{\alpha=x,y,z} \left\{ \frac{e^2}{8m_{e\alpha}c^2} \left\langle \left[a_\alpha(\mathbf{r}_e) - \frac{\partial \overline{\phi}}{\partial x_{e\alpha}} \right]^2 \right\rangle + \frac{e^2}{8m_{h\alpha}c^2} \left\langle \left[a_\alpha(\mathbf{r}_h) + \frac{\partial \overline{\phi}}{\partial x_{h\alpha}} \right]^2 \right\rangle \right\}. \tag{2.18}$$

At this point, we specify the z direction to be the direction of the magnetic field, and we choose the symmetric gauge so that $\mathbf{A} = (-\frac{1}{2}By, \frac{1}{2}Bx, 0)$. Then $\mathbf{a} = (-y, x, 0)$,

$$\gamma_2 = \min_{\overline{\phi}} \left\{ \frac{e^2}{8m_{ex}c^2} \left\langle \left[y_e + \frac{\partial \overline{\phi}}{\partial x_e} \right]^2 \right\rangle + \frac{e^2}{8m_{hx}c^2} \left\langle \left[y_h - \frac{\partial \overline{\phi}}{\partial x_h} \right]^2 \right\rangle + \frac{e^2}{8m_{ey}c^2} \left\langle \left[x_e - \frac{\partial \overline{\phi}}{\partial y_e} \right]^2 \right\rangle + \frac{e^2}{8m_{hy}c^2} \left\langle \left[x_h + \frac{\partial \overline{\phi}}{\partial y_h} \right]^2 \right\rangle + \frac{e^2}{8m_{ez}c^2} \left\langle \left(\frac{\partial \overline{\phi}}{\partial z_e} \right)^2 \right\rangle + \frac{e^2}{8m_{hz}c^2} \left\langle \left(\frac{\partial \overline{\phi}}{\partial z_h} \right)^2 \right\rangle \right\}. \tag{2.19}$$

In summary, the calculation of γ_2, the diamagnetic coefficient, proceeds in two steps. First, the expectation value of the zero-field Hamiltonian H_0 is minimized to find the best wave function χ, which is used to form the expectation values in Eqs. (2.17), (2.18), and (2.19). Then, the right-hand side of Eq. (2.19) is minimized with respect to the function $\overline{\phi}(\mathbf{r}_e, \mathbf{r}_h)$ to find the diamagnetic coefficient.

The calculation of the diamagnetic coefficient γ_2 is thus expressed in terms of finding the function $\overline{\phi}(\mathbf{r}_e, \mathbf{r}_h)$, which minimizes the expression on the right-hand side of Eq. (2.19).

B. Quantum well

Before considering the cases of the quantum wire and the quantum dot, we discuss the quantum well. This has been treated by Nash *et al.*[1] We consider a quantum well in a magnetic field with the field direction perpendicular to the quantum well plane. For the quantum well, the function $\overline{\phi}$ that minimizes the right-hand side of Eq. (2.19) can be found exactly.[12] It is

$$\overline{\phi} = -x_e y_h + x_h y_e. \tag{2.20}$$

The quantum well has translational invariance in the x-y plane, and so it might be expected that the canonical in-plane center-of-mass momenta P_X and P_Y would commute with the Hamiltonian (2.4). This is not the case at finite magnetic field. However, the center-of-mass momenta P_X and P_Y do commute with the transformed Hamiltonian (2.10):

$$[P_X, H'] = [P_Y, H'] = 0. \tag{2.21}$$

Additionally, if we denote by H_0, H_1', and H_2' terms in the Hamiltonian H' that are independent of magnetic field, linear in the field, and quadratic in the field, we find that

$$[H_0, H_1'] = 0. \tag{2.22}$$

This last point is what makes the transformation (2.20) exact. If we use perturbation theory to calculate the diamagnetic coefficient, we must treat H_2' in first order and H_1' in second order. However, since H_0 and H_1' commute, all matrix elements of H_1' between different eigenstates of H_0 will vanish, and hence the second-order contribution of H_1' vanishes. This greatly simplifies the calculation of the diamagnetic coefficient.

We have, then, that the diamagnetic coefficient for an exciton in a quantum well is given by

$$\gamma_2 = \frac{e^2}{8\mu c^2} \langle \rho^2 \rangle, \tag{2.23}$$

where the expectation value is with respect to the zero-field eigenstate (the eigenstate of H_0), and μ is the in-plane reduced mass of the exciton. The diamagnetic coefficient contains information about the zero-field properties of the exciton. In the case of the quantum well, Eq. (2.23) shows that the diamagnetic coefficient is a measure of the in-plane electron-hole separation.

C. Lateral confinement

In general, when there is lateral confinement, we cannot find exactly the function $\overline{\phi}$ that minimizes the right-hand side of Eq. (2.19). We can, however, choose a functional form for $\overline{\phi}$ with variational parameters. The parameters are determined by minimizing the energy, which implies minimizing the right-hand side of Eq. (2.19).

Consider the transformation generated by

$$\overline{\phi} = -\lambda_1 x_e y_h + \lambda_2 x_h y_e + \lambda_e x_e y_e - \lambda_h x_h y_h. \tag{2.24}$$

The first two terms are a generalization of Eq. (2.20). The third is a gauge transformation for the electron, and the fourth is a gauge transformation for the hole. The meaning of the λ's and their relationships in various geometries are summarized in Table I. Using this transformation, we have

TABLE I. The meaning of particular values of λ's. X and Y are the center-of-mass coordinates in the x and y directions, respectively.

λ_1	λ_2	λ_e	λ_h	
0	0	0	0	symmetric gauge
0	0	1	1	Landau gauge
1	1	0	0	relative electron-hole coordinates, used for quantum well
λ	λ	0	0	used for cylindrical quantum dot
λ_1	λ_2	$1-\lambda_2$	$1-\lambda_1$	condition for γ_2 to be independent of X
λ_1	λ_2	λ_1-1	λ_2-1	condition for γ_2 to be independent of Y
$1+\lambda$	$1-\lambda$	λ	$-\lambda$	condition for γ_2 to be independent of X and Y

$$\gamma_2=\min_{\lambda_1,\lambda_2,\lambda_e,\lambda_h}\frac{e^2}{8c^2}\left\{\left[\frac{(1-\lambda_e)^2}{m_{ey}}+\frac{\lambda_1^2}{m_{hy}}\right]\langle x_e^2\rangle+\left[\frac{(1+\lambda_e)^2}{m_{ex}}+\frac{\lambda_2^2}{m_{hx}}\right]\langle y_e^2\rangle-2\left[\frac{(1-\lambda_e)\lambda_2}{m_{ey}}+\frac{(1-\lambda_h)\lambda_1}{m_{hy}}\right]\langle x_e x_h\rangle\right.$$
$$\left.-2\left[\frac{(1+\lambda_e)\lambda_1}{m_{ex}}+\frac{(1+\lambda_h)\lambda_2}{m_{hx}}\right]\langle y_e y_h\rangle+\left[\frac{\lambda_2^2}{m_{ey}}+\frac{(1-\lambda_h)^2}{m_{hy}}\right]\langle x_h^2\rangle+\left[\frac{\lambda_1^2}{m_{ex}}+\frac{(1+\lambda_h)^2}{m_{hx}}\right]\langle y_h^2\rangle\right\}. \tag{2.25}$$

The following system of linear equations gives the values of λ_1, λ_2, λ_e, and λ_h, which determine the best result for the diamagnetic coefficient:

$$\begin{bmatrix} \frac{\langle x_e^2\rangle}{m_{hy}}+\frac{\langle y_h^2\rangle}{m_{ex}} & 0 & -\frac{\langle y_e y_h\rangle}{m_{ex}} & \frac{\langle x_e x_h\rangle}{m_{hy}} \\ 0 & \frac{\langle x_h^2\rangle}{m_{ey}}+\frac{\langle y_e^2\rangle}{m_{hx}} & \frac{\langle x_e x_h\rangle}{m_{ey}} & -\frac{\langle y_e y_h\rangle}{m_{hx}} \\ -\frac{\langle y_e y_h\rangle}{m_{ex}} & \frac{\langle x_e x_h\rangle}{m_{ey}} & \frac{\langle x_e^2\rangle}{m_{ey}}+\frac{\langle y_e^2\rangle}{m_{ex}} & 0 \\ \frac{\langle x_e x_h\rangle}{m_{hy}} & -\frac{\langle y_e y_h\rangle}{m_{hx}} & 0 & \frac{\langle x_h^2\rangle}{m_{hy}}+\frac{\langle y_h^2\rangle}{m_{hx}} \end{bmatrix}\begin{bmatrix}\lambda_1\\ \lambda_2\\ \lambda_e\\ \lambda_h\end{bmatrix}=\begin{bmatrix} \frac{\langle x_e x_h\rangle}{m_{hy}}+\frac{\langle y_e y_h\rangle}{m_{ex}} \\ \frac{\langle x_e x_h\rangle}{m_{ey}}+\frac{\langle y_e y_h\rangle}{m_{hx}} \\ \frac{\langle x_e^2\rangle}{m_{ey}}-\frac{\langle y_e^2\rangle}{m_{ex}} \\ \frac{\langle x_h^2\rangle}{m_{hy}}-\frac{\langle y_h^2\rangle}{m_{hx}} \end{bmatrix}. \tag{2.26}$$

In summary, the diamagnetic coefficient is calculated in the following way. First, the ground state of Hamiltonian (2.1) must be found. This is the ground-state exciton wave function in the absence of a magnetic field, and it can be found in any convenient way. Second, expectation values of the coordinates are calculated with respect to this state and used in Eq. (2.26) to find λ_1, λ_2, λ_e, and λ_h. Finally, these values are used in Eq. (2.25) to evaluate the diamagnetic coefficient. The values of λ_1 and λ_2 are seen to give information about the relative contributions of lateral confinement and Coulomb interaction to the diamagnetic coefficient.

III. SYMMETRY IN THE CONFINING POTENTIAL

In the previous section, we introduced four variational parameters in order to calculate the diamagnetic coefficient. Here, we will see that symmetries in the confining potential place constraints on these parameters, thereby reducing their number.

There are two situations in which simplifications arise. The first case is cylindrical symmetry along an axis parallel to the magnetic field. The second is translational symmetry in a direction perpendicular to the magnetic field.

A. Cylindrical symmetry

In the case of cylindrical symmetry, there is no mass anisotropy,

$$m_{ex}=m_{ey}\equiv m_e,$$
$$m_{hx}=m_{hy}\equiv m_h, \tag{3.1}$$

and expectation values of x coordinates at zero magnetic field must be the same as expectation values of y coordinates:

$$\langle x_e^2\rangle=\langle y_e^2\rangle,$$
$$\langle x_h^2\rangle=\langle y_h^2\rangle, \tag{3.2}$$
$$\langle x_e x_h\rangle=\langle y_e y_h\rangle.$$

Solving Eq. (2.26) under these conditions leads to the constraints

$$\lambda_1=\lambda_2\equiv\lambda,$$
$$\lambda_e=\lambda_h=0, \tag{3.3}$$

so that with cylindrical symmetry, only one variational parameter λ is needed. The expression for λ is

$$\lambda=\frac{\langle\rho_e^2\rangle+\langle\rho_h^2\rangle-\langle\rho^2\rangle}{2\dfrac{\mu}{m_h}\langle\rho_e^2\rangle+2\dfrac{\mu}{m_e}\langle\rho_h^2\rangle}, \tag{3.4}$$

with $1/\mu=1/m_e+1/m_h$, $\langle\rho_e^2\rangle=\langle x_e^2\rangle+\langle y_e^2\rangle$, $\langle\rho_h^2\rangle=\langle x_h^2\rangle+\langle y_h^2\rangle$, and $\langle\rho^2\rangle=\langle(x_e-x_h)^2\rangle+\langle(y_e-y_h)^2\rangle$.

Expression (3.4) shows that λ is a measure of the relative influence of lateral confinement of the electron and hole and electron-hole Coulomb interaction on the diamagnetic coefficient. If the motion of the electron and hole were uncorrelated by the electron-hole interaction, then $\langle\rho^2\rangle=\langle\rho_e^2\rangle+\langle\rho_h^2\rangle$, so $\lambda=0$, and the geometry alone determines the diamagnetic coefficient. At the other extreme, with no lateral confinement, $\langle\rho_e^2\rangle\to\infty$ and $\langle\rho_h^2\rangle\to\infty$, so $\lambda=1$, and the relative (in-plane) electron-hole separation alone determines the diamagnetic coefficient through Eq. (2.23).

Using the value of λ from Eq. (3.4), we find that the diamagnetic coefficient for a structure with cylindrical symmetry can be written

$$\gamma_2=\frac{e^2}{8c^2}\frac{\lambda}{\mu}\langle\rho^2\rangle+\frac{e^2}{8c^2}\left[\frac{1}{m_e}+\frac{\lambda^2}{m_h}-\frac{\lambda}{\mu}\right]\langle\rho_e^2\rangle$$

$$+\frac{e^2}{8c^2}\left[\frac{1}{m_h}+\frac{\lambda^2}{m_e}-\frac{\lambda}{\mu}\right]\langle\rho_h^2\rangle. \tag{3.5}$$

The case of cylindrical symmetry illustrates most simply that in confined structures the lateral confinement and the Coulomb interaction compete to determine the exciton diamagnetic coefficient. In the strong lateral confinement regime, γ_2 is a measure of lateral confinement of the electron and the hole. In the weak confinement regime, γ_2 is a measure of in-plane electron-hole separation. The value of λ serves to characterize the relative strength of lateral confinement and Coulomb interaction, with $\lambda=0$ corresponding to the strong-confinement limit, and $\lambda=1$ corresponding to the weak-confinement limit.

B. Translational symmetry

Let us choose the x axis to be along the direction of translational symmetry. This would be the case in, for example, a quantum wire. Then, the diamagnetic coefficient must be independent of X, the exciton center-of-mass coordinate in the x direction. This leads to the following constraints:

$$\lambda_e=1-\lambda_2, \tag{3.6}$$

$$\lambda_h=1-\lambda_1, \tag{3.7}$$

so that in the case of translational symmetry, two variational parameters are needed. We find λ_1 and λ_2 from the linear equations

$$\begin{bmatrix}\dfrac{\langle x^2\rangle}{m_{hy}}+\dfrac{\langle y_h^2\rangle}{\mu_x} & \dfrac{\langle y_e y_h\rangle}{\mu_x}\\ \dfrac{\langle y_e y_h\rangle}{\mu_x} & \dfrac{\langle x^2\rangle}{m_{ey}}+\dfrac{\langle y_e^2\rangle}{\mu_x}\end{bmatrix}\begin{bmatrix}\lambda_1\\ \lambda_2\end{bmatrix}=2\begin{bmatrix}\dfrac{\langle y_h^2\rangle}{m_{hx}}+\dfrac{\langle y_e y_h\rangle}{m_{ex}}\\ \dfrac{\langle y_e^2\rangle}{m_{ex}}+\dfrac{\langle y_e y_h\rangle}{m_{hx}}\end{bmatrix}, \tag{3.8}$$

where $1/\mu_x=1/m_{ex}+1/m_{hx}$ and $\langle x^2\rangle=\langle(x_e-x_h)^2\rangle$. Using these values of λ_1 and λ_2, we find that the diamagnetic coefficient is given by

$$\gamma_2=\frac{e^2}{8c^2}\left\{\left[\frac{\lambda_2^2}{m_{ey}}+\frac{\lambda_1^2}{m_{hy}}\right]\langle x^2\rangle+\left[\frac{(2-\lambda_2)^2}{m_{ex}}+\frac{\lambda_2^2}{m_{hx}}\right]\langle y_e^2\rangle\right.$$

$$-2\left[\frac{(2-\lambda_2)\lambda_1}{m_{ex}}+\frac{(2-\lambda_1)\lambda_2}{m_{hx}}\right]\langle y_e y_h\rangle$$

$$\left.+\left[\frac{\lambda_1^2}{m_{ex}}+\frac{(2-\lambda_1)^2}{m_{hx}}\right]\langle y_h^2\rangle\right\}. \tag{3.9}$$

Once again we see that the diamagnetic coefficient is determined by the interplay of the lateral confinement and the Coulomb interaction.

IV. QUANTUM WELL, WIRE, AND DOT STRUCTURES

In this section we apply the method developed above to discuss exciton diamagnetic coefficients in quantum wells, quantum wires, and quantum dots. Here it is our intention to illustrate the effects of confinement and dimensionality on the exciton properties. For this discussion we use models of these systems. We take the electrons and holes to exist in isotropic bands with masses $m_e=0.0665$ and $m_h=0.35$ in both the nanostructure and in the barrier material, and we take the background dielectric constant to be 12.5 in each material. The effects of confinement are represented by potential barriers for the carriers where 65% of the total offset is in the conduction band and 35% is in the valence band. In separate work[11,14] we have compared the results of such calculations with the most recent, detailed data for excitonic diamagnetic shifts and binding energies in quantum wires and quantum dots. The systems studied in that work were lithographic $In_xGa_{1-x}As/GaAs$ structures with widely varying sizes and potential barriers.

As pointed out above, we must first find the ground-state exciton wave function in the absence of a magnetic field. It should be noted that the formulation developed here is applicable using any method for calculating the zero-field wave function. Here we choose a variational technique based on a two-parameter nonseparable variational wave function[13]

$$\Psi(\mathbf{r}_e,\mathbf{r}_h)=f_e(\mathbf{r}_e)f_h(\mathbf{r}_h)\exp\{-\sqrt{\alpha^2[(x_e-x_h)^2+(y_e-y_h)^2]+\beta^2(z_e-z_h)^2}\}, \tag{4.1}$$

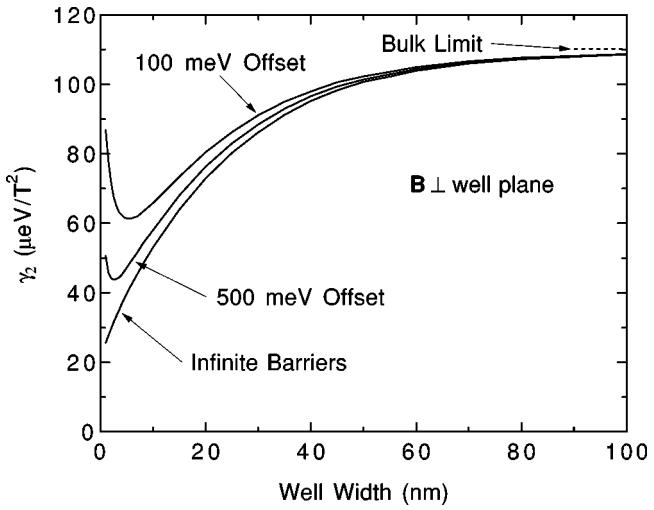

FIG. 1. Exciton diamagnetic coefficient as a function of quantum well width. The magnetic field is perpendicular to the quantum well plane. The total (electron+hole) potential offsets are 100 meV, 500 meV, and infinite. The bulk limit of 110.2 μeV/T^2 is shown as a dashed line.

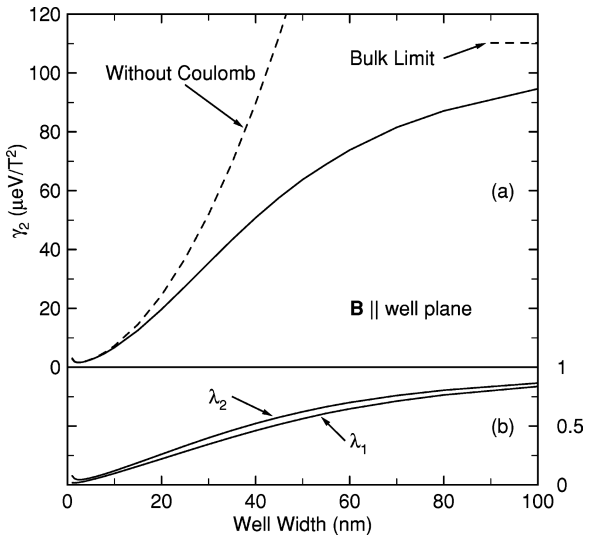

FIG. 2. Quantum well with magnetic field parallel to the well plane. The total (electron+hole) potential offset is 1000 meV. (a) Exciton diamagnetic coefficient as a function of well width. The bulk limit of 110.2 μeV/T^2 is shown as a dashed line. The diamagnetic coefficient in the absence of the Coulomb interaction is also shown as a dashed line. (b) Values of variational parameters λ_1 and λ_2 for this structure.

in which α and β are the variational parameters. The functions $f_e(\mathbf{r}_e)$ and $f_h(\mathbf{r}_h)$ are the ground-state single-particle wave functions for a confined electron or hole in the structure. The parameter β goes with the coordinate perpendicular to the well plane in the case of the quantum well and parallel to the wire direction in the case of the quantum wire. The quantum dot studied here is taken to have full rotational symmetry, so a single parameter $\alpha=\beta$ is used in that case.

Two magnetic-field orientations are studied for the quantum well, that of the field perpendicular to the well plane and that of the field parallel to the well plane. Figure 1 shows the calculated diamagnetic coefficient for an exciton in a quantum well with magnetic field perpendicular to the well plane. In this case, Eq. (2.23) is used to evaluate γ_2, and we do not need the variational parameters introduced in Sec. II C. Results are shown for three potential offsets, which cover a wide range. Except for very thin wells, there is a weak dependence on potential offset. The basic trend is that γ_2 decreases with decreasing structure size, which indicates a reduction in the in-plane electron-hole separation. In all cases, the bulk limit of 110.2 μeV/T^2 is approached at large well widths. For very thin wells (smaller than $\sim$5 nm), the structures with finite potential confinement show an increase in γ_2 with decreasing well width, which is an indication that a significant part of the exciton wave function is extending into the barrier regions. For such thin wells the diamagnetic shifts approach those of the bulk barrier materials. In the case of infinite barriers, the ideal 2D limit $(\gamma_2)_{2D}=\frac{3}{16}(\gamma_2)_{3D}$ of 20.7 μeV/T^2 is reached. For the case of the quantum well with magnetic field perpendicular to the well plane, the diamagnetic coefficient is entirely a result of the electron-hole Coulomb interaction because there is no lateral confinement. In the absence of the Coulomb interaction, we find Landau levels for electrons and holes with linear magnetic-field dependences, and no quadratic shift.

Figure 2 shows the calculated diamagnetic coefficient for an exciton in a quantum well with magnetic field parallel to the well plane. In this case, the results of Sec. III B apply with two variational parameters, λ_1 and λ_2, required to calculate γ_2. Here the diamagnetic coefficient is lower than that in the corresponding case with perpendicular field because we now have the influence of lateral confinement in addition the effect of the Coulomb interaction. The λ's required for the calculation of γ_2 for each geometry and magnetic-field direction are listed in Table II for both the usual case including the Coulomb interaction and also for the case of ignoring the Coulomb interaction.

The value of γ_2 in the absence of the Coulomb interaction is shown in Fig. 2 with a dashed line, and it increases with-

TABLE II. Variational parameters used in the calculation of γ_2 for quantum well, cylindrical quantum wire, and spherical quantum dot geometries. For the quantum well with magnetic field perpendicular to the well plane in the absence of the Coulomb interaction there is no diamagnetic shift, but rather Landau levels.

Structure	With Coulomb interaction	Without Coulomb interaction
well, $\mathbf{B}\perp$well plane	none	n/a
well, $\mathbf{B}\parallel$well plane	λ_1, λ_2	none
wire, $\mathbf{B}\parallel$wire axis	λ	none
wire, $\mathbf{B}\perp$wire axis	λ_1, λ_2	none
dot	λ	none

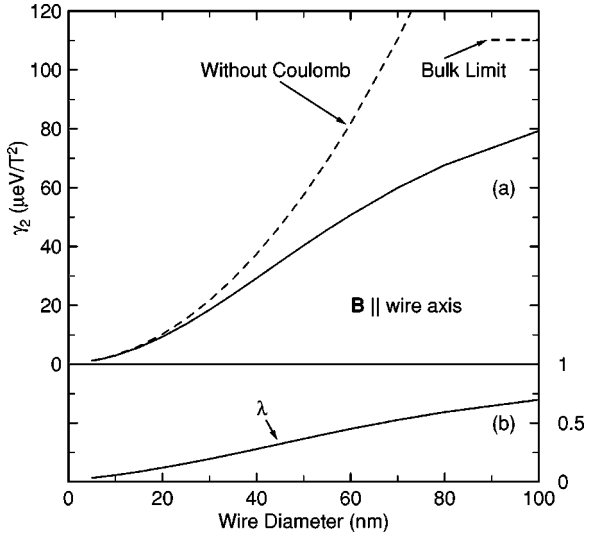

FIG. 3. Quantum wire with magnetic field parallel to the wire axis. The total (electron+hole) potential offset is 1000 meV. (a) Exciton diamagnetic coefficient as a function of wire diameter. The bulk limit of 110.2 μeV/T^2 is shown as a dashed line. The diamagnetic coefficient in the absence of the Coulomb interaction is also shown as a dashed line. (b) Values of variational parameter λ for this structure.

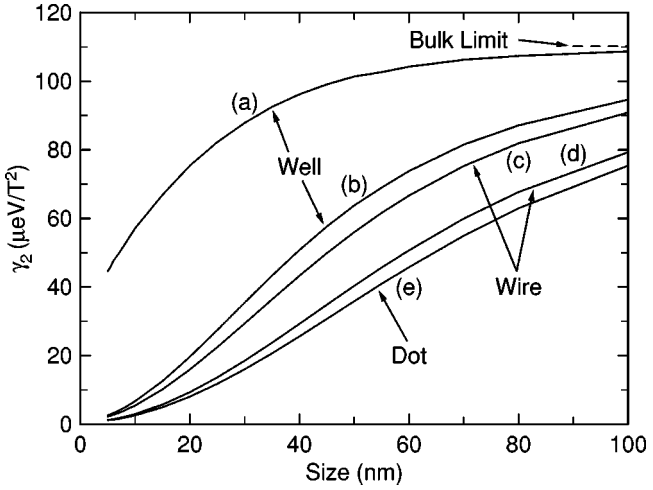

FIG. 4. Comparison of diamagnetic coefficient for quantum well, cylindrical quantum wire, and spherical quantum dot. Size (nm) refers to well width, wire diameter, or dot diameter. The total (electron+hole) potential offset is 1000 meV. (a) $\mathbf{B}\perp$ well plane. (b) $\mathbf{B}\|$well plane. (c) $\mathbf{B}\perp$ wire axis. (d) $\mathbf{B}\|$wire axis. (e) Spherical quantum dot.

out bound as well width grows. This is because in the absence of the Coulomb interaction, γ_2 depends only on expectation values of the lateral single-particle coordinates, which increase with well width. This is shown in Eq. (3.9) with $\lambda_1=\lambda_2=0$. In this case, the range of magnetic field over which the energy shift is quadratic shrinks with increasing structure size, ending in Landau levels in the bulk. For thin wells, the diamagnetic coefficients with and without the Coulomb interaction converge, showing that γ_2 is not sensitive to the Coulomb interaction in the strong-confinement limit.

The values of λ_1 and λ_2 for the calculations that include the Coulomb interaction are shown in part (b) of the figure. The small values for thin wells indicate that γ_2 is acting as a measure of lateral confinement in the thin well regime, whereas the values approaching 1 for large wells imply that γ_2 is a measure of in-plane electron-hole separation in the large well regime.

Figure 3 shows the calculated diamagnetic coefficient for an exciton in a quantum wire with magnetic field parallel to the wire axis. In this case, there is cylindrical symmetry about the wire axis, and the results of Sec. III A apply with one variational parameter λ required to calculate γ_2. Here the diamagnetic coefficient is lower than that in the quantum well with either field direction, due to the stronger lateral confinement. The value of λ for the calculation including the Coulomb interaction is shown in part (b) of the figure. The small values for thin wires indicate that γ_2 is acting as a measure of lateral confinement in the thin well regime, while the values approaching 1 for large wires imply that γ_2 is a measure of in-plane electron-hole separation in the large wire regime.

Figure 4 shows a comparison of all of the structures and magnetic-field directions studied. The lower-dimensional structures have lower diamagnetic coefficients, implying smaller in-plane electron-hole separations for the larger-size structures and stronger lateral confinement for the smaller-size structures. In all cases the diamagnetic coefficient decreases with decreasing size.

In conclusion, we have presented a method for calculating the diamagnetic coefficient of an exciton in a semiconductor nanostructure. We have introduced a generalized gauge transformation in the calculation of the exciton energy in confined systems. This transformation furnishes parameters that provide measures of the role of lateral confinement and of Coulomb interaction in the diamagnetic shift.

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APPENDIX A: DERIVATION OF EXPRESSION FOR γ_2

We begin with Eq. (2.12). To simplify the notation, define

$$W=\sum_{i=e,h}\sum_{\alpha=x,y,z}\frac{\left[\frac{q_i}{c}A_\alpha(\mathbf{r}_i)+\hbar\frac{\partial\phi}{\partial x_{i\alpha}}\right]^2}{2m_{i\alpha}}. \tag{A1}$$

Then,

$$\langle H'\rangle=\langle H_0\rangle+\langle W\rangle. \tag{A2}$$

Now, $\langle H'\rangle$ depends on the magnetic field B in two ways. First, W depends explicitly on B through the vector potential $\mathbf{A}$ and the gauge function ϕ. Second, the expectation value is with respect to the real wave function χ, which depends on B through the parameters α_i. The required first and second derivatives of $\langle H'\rangle$ with respect to B are

$$\frac{d\langle H'\rangle}{dB}=\left\langle\frac{dW}{dB}\right\rangle+\sum_i\frac{\partial\langle H'\rangle}{\partial\alpha_i}\frac{d\alpha_i}{dB} \tag{A3}$$

and

$$\frac{d^2\langle H'\rangle}{dB^2}=\left\langle\frac{d^2W}{dB^2}\right\rangle+2\sum_i\frac{\partial}{\partial\alpha_i}\left\langle\frac{dW}{dB}\right\rangle\frac{d\alpha_i}{dB}+\sum_i\sum_{i'}\frac{\partial^2\langle H'\rangle}{\partial\alpha_i\partial\alpha_{i'}}\frac{d\alpha_i}{dB}\frac{d\alpha_{i'}}{dB}+\sum_i\frac{\partial\langle H'\rangle}{\partial\alpha_i}\frac{d^2\alpha_i}{dB^2}. \tag{A4}$$

1. Calculation of coefficients

We are now ready to calculate the coefficients in expansion (2.13) by evaluating $\langle H'\rangle$ and its derivatives at $B=0$. Evaluating Eq. (2.12) at $B=0$ gives

$$[\langle H'\rangle]_{B=0}=[\langle H_0\rangle]_{B=0}+\sum_{i=e,h}\sum_{\alpha=x,y,z}\frac{\hbar^2}{2m_{i\alpha}}\left[\left\langle\left(\frac{\partial\phi_0}{\partial x_{i\alpha}}\right)^2\right\rangle\right]_{B=0}. \tag{A5}$$

Since the second term above can give only a positive contribution, ϕ_0 can be at most a constant, which corresponds to an arbitrary phase for the entire wave function, which we set to zero,

$$\phi_0=0, \tag{A6}$$

and so

$$[\langle H'\rangle]_{B=0}=[\langle H_0\rangle]_{B=0}. \tag{A7}$$

Next, evaluating Eq. (A3) at $B=0$ gives

$$\left[\frac{d\langle H'\rangle}{dB}\right]_{B=0}=\left[\left\langle\frac{dW}{dB}\right\rangle\right]_{B=0}+\sum_i\left[\frac{\partial\langle H'\rangle}{\partial\alpha_i}\right]_{B=0}\left[\frac{d\alpha_i}{dB}\right]_{B=0}. \tag{A8}$$

We can simplify each part of this expression. From Eq. (2.15), we have that

$$\left[\frac{d\alpha_i}{dB}\right]_{B=0}=\alpha_i^{(1)}. \tag{A9}$$

Next, we notice that the functional dependence of $\langle H'\rangle$ on α_i is the same as the functional dependence of $[\langle H'\rangle]_{B=0}$ on $\alpha_i^{(0)}$ for the portion of $\langle H'\rangle$ that remains when B is set to zero. This means that

$$\left[\frac{\partial\langle H'\rangle}{\partial\alpha_i}\right]_{B=0}=\frac{\partial}{\partial\alpha_i^{(0)}}[\langle H'\rangle]_{B=0}. \tag{A10}$$

Finally, since $\mathbf{A}$ is linear in B and $\phi_0=0$, W has only quadratic and higher even powers of B, so

$$\left[\left\langle\frac{dW}{dB}\right\rangle\right]_{B=0}=0. \tag{A11}$$

Therefore, Eq. (A8) simplifies to

$$\left[\frac{d\langle H'\rangle}{dB}\right]_{B=0}=\sum_i\alpha_i^{(1)}\frac{\partial}{\partial\alpha_i^{(0)}}[\langle H'\rangle]_{B=0}. \tag{A12}$$

Evaluating the second derivative of $\langle H'\rangle$ at $B=0$ gives

$$\left[\frac{d^2\langle H'\rangle}{dB^2}\right]_{B=0}=\left[\left\langle\frac{d^2W}{dB^2}\right\rangle\right]_{B=0}+2\sum_i\alpha_i^{(1)}\left[\frac{\partial}{\partial\alpha_i}\left\langle\frac{dW}{dB}\right\rangle\right]_{B=0}+\sum_i\sum_{i'}\alpha_i^{(1)}\alpha_{i'}^{(1)}\left[\frac{\partial^2\langle H'\rangle}{\partial\alpha_i\partial\alpha_{i'}}\right]_{B=0}+\sum_i\left[\frac{\partial\langle H'\rangle}{\partial\alpha_i}\right]_{B=0}\left[\frac{d^2\alpha_i}{dB^2}\right]_{B=0}. \tag{A13}$$

We obtain simplifying expressions that are similar to those used for the first derivative above and are

$$\left[\frac{d^2\alpha_i}{dB^2}\right]_{B=0}=2\alpha_i^{(2)}, \tag{A14}$$

$$\left[\frac{\partial}{\partial\alpha_i}\left\langle\frac{dW}{dB}\right\rangle\right]_{B=0}=\frac{\partial}{\partial\alpha_i^{(0)}}\left[\left\langle\frac{dW}{dB}\right\rangle\right]_{B=0}=0. \tag{A15}$$

Substituting these, we have

$$\left[\frac{1}{2}\frac{d^2\langle H'\rangle}{dB^2}\right]_{B=0}=\frac{1}{2}\left[\left\langle\frac{d^2W}{dB^2}\right\rangle\right]_{B=0}+\frac{1}{2}\sum_i\sum_{i'}\alpha_i^{(1)}\alpha_{i'}^{(1)}\frac{\partial^2}{\partial\alpha_i^{(0)}\partial\alpha_{i'}^{(0)}}\times[\langle H'\rangle]_{B=0}+\sum_i\alpha_i^{(2)}\frac{\partial}{\partial\alpha_i^{(0)}}[\langle H'\rangle]_{B=0}. \tag{A16}$$

2. Minimization of coefficients

The coefficients that we just calculated must now be minimized with respect to $\alpha_i^{(n)}$ and ϕ_i to give E_0, γ_1, and γ_2 as in Eq. (2.16).

$[\langle H'\rangle]_{B=0}$ depends only on $\alpha_i^{(0)}$,

$$\frac{\partial}{\partial\alpha_i^{(0)}}[\langle H'\rangle]_{B=0}=0; \tag{A17}$$

$[d\langle H'\rangle/dB]_{B=0}$ depends only on $\alpha_i^{(0)}$ and $\alpha_i^{(1)}$,

$$\frac{\partial}{\partial\alpha_i^{(0)}}\left[\frac{d\langle H'\rangle}{dB}\right]_{B=0}=0, \tag{A18}$$

$$\frac{\partial}{\partial\alpha_i^{(1)}}\left[\frac{d\langle H'\rangle}{dB}\right]_{B=0}=0. \tag{A19}$$

This results in the two sets of equations:

$$\sum_{i'} \alpha_{i'}^{(1)} \frac{\partial^2}{\partial \alpha_i^{(0)} \partial \alpha_{i'}^{(0)}} [\langle H' \rangle]_{B=0} = 0, \tag{A20}$$

$$\frac{\partial}{\partial \alpha_i^{(0)}} [\langle H' \rangle]_{B=0} = 0. \tag{A21}$$

Note that Eq. (A21) is the same as Eq. (A17). $[d^2\langle H' \rangle / dB^2]_{B=0}$ depends on $\alpha_i^{(0)}$, $\alpha_i^{(1)}$, $\alpha_i^{(2)}$, and ϕ_1:

$$\frac{\partial}{\partial \alpha_i^{(0)}} \left[\frac{1}{2} \frac{d^2\langle H' \rangle}{dB^2} \right]_{B=0} = 0, \tag{A22}$$

$$\frac{\partial}{\partial \alpha_i^{(1)}} \left[\frac{1}{2} \frac{d^2\langle H' \rangle}{dB^2} \right]_{B=0} = 0, \tag{A23}$$

$$\frac{\partial}{\partial \alpha_i^{(2)}} \left[\frac{1}{2} \frac{d^2\langle H' \rangle}{dB^2} \right]_{B=0} = 0, \tag{A24}$$

$$\frac{\partial}{\partial \alpha_i^{(0)}} \left[\frac{d^2\langle H' \rangle}{dB^2} \right]_{B=0} = 0, \tag{A25}$$

$$\sum_{i'} \alpha_{i'}^{(1)} \frac{\partial^2}{\partial \alpha_i^{(0)} \partial \alpha_{i'}^{(0)}} [\langle H' \rangle]_{B=0} = 0, \tag{A26}$$

$$\frac{\partial}{\partial \alpha_i^{(0)}} [\langle H' \rangle]_{B=0} = 0. \tag{A27}$$

Note that Eq. (A27) is the same as Eq. (A17) and that Eq. (A26) is the same as Eq. (A20). Putting all of this together, we find

$$\gamma_2 = \min_{\phi_1} \frac{1}{2} \left[\left\langle \frac{d^2 W}{dB^2} \right\rangle \right]_{B=0}. \tag{A28}$$

Evaluating this equation with Eq. (A1) gives the desired result, Eq. (2.17).

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