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Dressed-band approach and Coulomb corrections to the light-induced exciton Stark shift

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In the present work, we perform a comparison of theoretical approaches involving Coulomb-interaction corrections within the Hartree–Fock approximation and the renormalized dressed-band scheme in the large detuning limit. We focus on the well-studied optical Stark shift of the exciton peak in bulk and GaAs–(Ga,Al)As semiconductor quantum wells. It is argued that the Hartree–Fock scheme has severe limitations concerning its application to real experimental situations, even in the simplest laser field–perturbative regime. It is also shown, through a comparison between experiments and a three-band Kane-dressed GaAs–(Ga,Al)As quantum well calculation, that a proper treatment of band structure and confinement effects due to the quantum well is of fundamental importance in a theoretical understanding of Stark shift experimental measurements, and that the renormalized dressed-band approach is a very convenient tool to treat, in the large detuning limit, processes involving the laser–semiconductor interaction in low-dimensional heterostructures.
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I. INTRODUCTION

Recently, the effects of the laser field–semiconductor interaction on the electronic, impurity, and optical properties of semiconductor heterostructures, such as quantum wells and quantum dots, have been studied within an extended dressed-atom approach,[1] i.e., within a laser dressed-band formalism.[2–5] In this simple and straightforward scheme, it is possible to incorporate the laser effects through a renormalization of the semiconductor energy gap, and conduction/valence effective masses. Moreover, it may be applied to treat a variety of optoelectronic physical processes and provides an adequate indication of the laser effects on any low-dimensional semiconductor heterostructure system for which the effective-mass approximation is a good physical description. Of course, a proper understanding of the physics involved in the laser–semiconductor interaction is of paramount importance in the area of optoelectronic devices. The laser dressed-band approach has proved useful in the study of several physical situations, such as the optical excitonic Stark shifts and laser-induced shifts in shallow-impurity states in GaAs–(Ga,Al)As quantum wells (QWs) and quantum dots under applied magnetic fields.[4,5] The renormalized dressed-band scheme is nonperturbative in the field and justified if the laser is tuned far below any resonances as in this case many-body effects are small corrections to the one-body approximation. Also, if the laser detuning δ is much larger than the Rabi energy Λ_0, the linear (in the field intensity) regime prevails, and the usual perturbative results are recovered. The inclusion of the Coulomb corrections due to the electron–hole ($e-h$) interaction has been considered in the weak-field limit, within the Hartree–Fock approximation[6–8] or within a perturbative many-body diagramatic technique,[9] to study the exciton optical Stark shift in bulk systems. As discussed below, even for bulk systems and under these approximations the problem is already quite involved and the applications of the solutions have severe limitations. Of course, a treatment which includes Coulomb and laser-induced effects on excitons or impurities under magnetic fields in low-dimensional semiconductor heterostructures would be quite a formidable task even in the field-perturbative regime.

The purpose of the present work is to perform a comparison of theoretical approaches involving Coulomb-interaction corrections and the renormalized dressed-band scheme. In the case of the well studied problem of the exciton optical Stark shift,[6–9] both laser and Coulomb effects on the exciton binding energies may be incorporated within the renormalized-mass scheme through a summation of ladder diagrams associated with laser-dressed $e-h$ bubbles built from laser-dressed $e-h$ pairs in the presence of the Coulomb interaction.[4] In what follows we restrict the discussion to the Hartree–Fock (HF) approximation [within perturbation theory (PT)] since further correlation effects in the exciton–exciton interaction cannot be exactly calculated even in the field-perturbative and large-detuning limits.[9] We also briefly discuss the equivalence between the HF treatment by

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Schmitt-Rink *et al.*,[6] Ell *et al.*,[7] and Haug and Koch[8] and the diagramatic approach by Combescot.[9] Moreover, since these calculations are restricted to bulk systems, whereas most experiments are concerned with the observation of the optical Stark shifts of excitons in GaAs–(Ga,Al)As QWs, we compare them with the renormalized-mass dressed-band calculations for both bulk and semiconductor QWs. It is shown that a realistic description of the semiconductor band structure and a proper consideration of the confinement effects of the QW are of fundamental importance. In Sec. II we present a brief review of the renormalized effective-mass approach and of the HF calculations. Section III is dedicated to results and discussions. Conclusions are in Sec. IV and the Appendices are dedicated to the calculation of the HF terms in the large detuning limit.

II. THE LASER-DRESSED AND COULOMB CORRECTIONS WITHIN THE TWO-BAND SEMICONDUCTOR MODEL

A. The dressed-band approximation

We adopt a GaAs two-band model semiconductor in the **k.p** approximation interacting with a laser field, and take the matrix elements of the momentum operator as isotropic. The effect of a homogeneous laser field in the two-band model structure may be obtained from the Hamiltonian[2,3]

$$H=H_0+\hbar\omega a^+a+\frac{e}{m_0c}A_\omega\hat{p}.\hat{\epsilon}(a^++a), \tag{1}$$

where H_0 is the diagonal one-electron two-band matrix, and $a^+(a)$ is the creation (annihilation) photon operator associated with the laser mode of frequency ω and polarization $\hat{\epsilon}$. From the diagonalization of the Hamiltonian, one obtains[2,3] the associated laser-dressed conduction $(+)$ and valence $(-)$ electronic bands, i.e.,

$$\epsilon_\pm=\frac{\epsilon_g\pm\hbar\omega}{2}\pm\frac{1}{2}\sqrt{4\Lambda_0^2+\left(\delta+\frac{2\Lambda_0^2}{\Lambda_1}\right)^2}+\frac{\hbar^2k^2}{2m_\pm}, \tag{2}$$

and corresponding renormalized effective masses $m_\pm$ (see Brandi *et al.*[2,3]). In the above expression, ϵ_g is the semiconductor energy gap, δ is the laser detuning given by $\delta=\epsilon_g-\hbar\omega$, and $\Lambda_1=2\epsilon_g-\delta$. The characteristic energy associated to the laser–semiconductor interaction is related to

$$\Lambda_0=\left(\frac{eA_0|p|}{2m_0c}\right),$$

the Rabi energy.[1–3]

Note that the GaAs semiconductor energy gap is dressed by laser effects, and is given by the $k=0$ difference between the above renormalized conduction and valence electronic bands

$$\tilde{\epsilon}_g=\epsilon_g-\delta+\sqrt{4\Lambda_0^2+\left(\delta+\frac{2\Lambda_0^2}{\Lambda_1}\right)^2}. \tag{3}$$

The laser-dressed renormalized two-band model results corresponds to the $1s$-like exciton-peak shift given by

$$\Sigma_R=(\tilde{\epsilon}_g-\epsilon_g)-[E_0(I)-E_0], \tag{4}$$

where E_0 is the bulk three-dimensional (3D) exciton Rydberg, and $E_0(I)$ is the dressed-laser 3D exciton binding energy calculated with the dressed conduction/valence masses.

The above equations provide the framework for calculating laser effects on semiconductor systems within the two-band picture. The present renormalized effective-mass approach, valid within the one-particle picture and for a laser tuned far from any resonances, may be used to give an indication of the laser effects on any semiconductor heterostructure for which the effective-mass approximation is a good physical description. In what follows we investigate the laser effects on the ground-state exciton energies in both bulk GaAs and GaAs–(Ga,Al)As QWs. Far from resonances, the incorporation of the laser effects through the renormalized effective masses leads to a straightforward calculation of the exciton properties[4] following, for example, a simple variational scheme such as that detailed by Greene *et al.*[10]

B. Coulomb corrections within the Hartree–Fock approximation

Within the two-band HF approximation and taking Coulomb corrections perturbatively into account,[6–9] one may show that the weak-field limit of the Stark shift of the $1s$-like exciton peak is given by

$$\Sigma_{1s}=\Pi_{1s}+\Delta_{1s}, \tag{5}$$

where the Π_{1s} contribution is (see Appendices)

$$\Pi_{1s}=\frac{2\Lambda_0^2}{\delta}\left[1+2\sqrt{\frac{E_0}{\delta}}+(4\ln 2-1)\frac{E_0}{\delta}+\ldots\right], \tag{6}$$

whereas the corresponding Δ_{1s} contribution results in (cf. Appendices)

$$\Delta_{1s}=\frac{2\Lambda_0^2}{\delta}\left[\sqrt{\frac{E_0}{\delta}}+(4-4\ln 2)\frac{E_0}{\delta}+\ldots\right]. \tag{7}$$

Therefore, in the weak-field limit, the $1s$-exciton Stark shift is given by

$$\Sigma_{1s}=\frac{2\Lambda_0^2}{\delta}\left[1+3\sqrt{\frac{E_0}{\delta}}+3\frac{E_0}{\delta}+\ldots\right]. \tag{8}$$

Here we should mention that the result we have obtained for the Δ_{1s} term differs from

$$\Delta_{1s}=\frac{2\Lambda_0^2}{\delta}\left[\sqrt{\frac{E_0}{\delta}}+(6-4\ln 2)\frac{E_0}{\delta}+\ldots\right], \tag{9}$$

as obtained by Combescot[9] (see details of the present calculation in the Appendices). Although they have used equations which are basically those defined for $\Sigma_{\lambda\lambda}$, Schmitt–Rink *et al.*,[6] Ell *et al.*,[7] Haug and Koch,[8] and von Lehmen *et al.*,[11] in order to calculate the shift of the $1s$-exciton peak, have assumed additional approximations of which the limitations have been discussed by Combescot[9] and Zimmermann.[12]

III. RESULTS AND DISCUSSION

The purpose of this section is to compare the results of the renormalized dressed-band scheme with some existing HF calculations. In Fig. 1 we present the exciton $1s$ peak

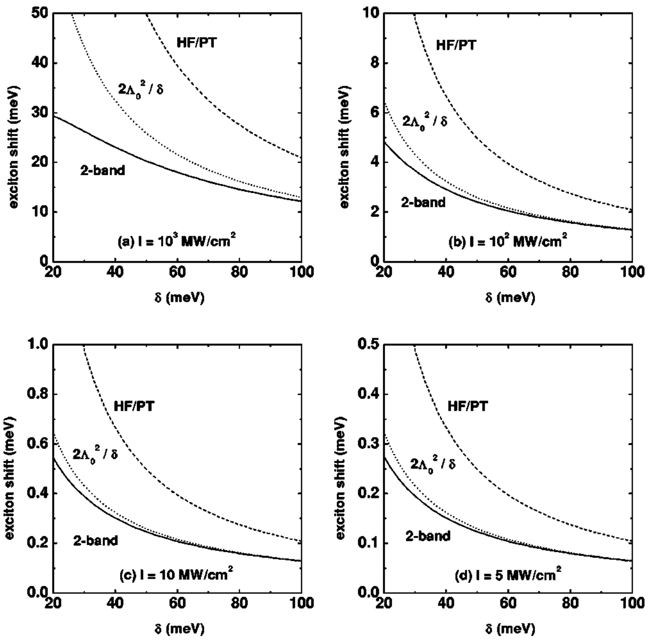

FIG. 1. Stark shifts of the 1*s*-like exciton peak for bulk GaAs, as functions of the laser detuning, within the two-band Callaway model (full curves) and Hartree–Fock perturbation theory (HF–PT) approach (dashed lines). Also shown are the results of the zero-order term of the perturbative calculations (dotted lines). Results are shown for different laser intensities.

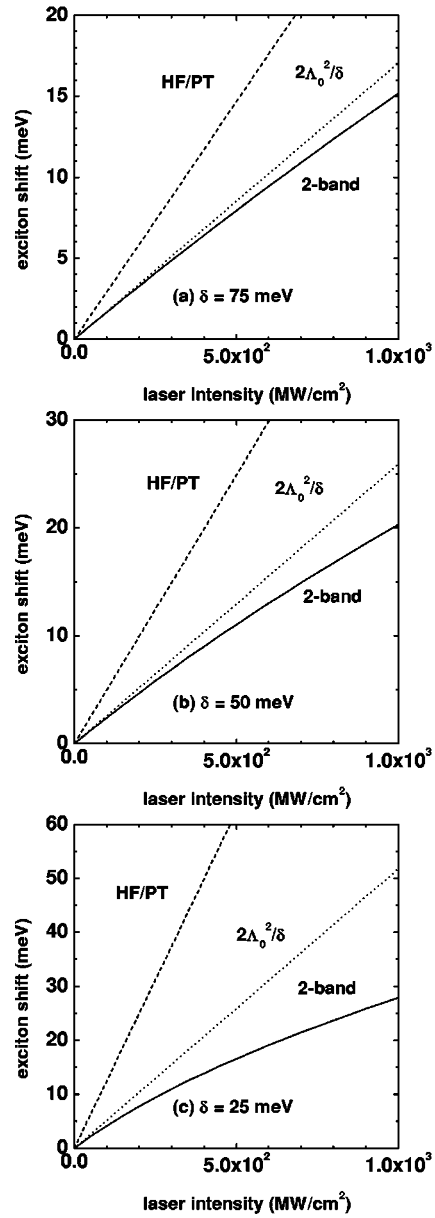

FIG. 2. Exciton shifts of the 1*s*-like exciton peak for bulk GaAs, as functions of the laser intensity for different values of the laser detuning within the two-band model (full curves) and HF–PT (dashed lines). Also shown are the results of the zero-order term of the perturbative calculations (dotted lines).

shift for bulk GaAs as a function of the laser detuning. As expected, it is clear from Fig. 1 the importance of considering a nonperturbative approach in the field intensity, as the laser intensities increase and the detuning decreases. In particular, in Fig. 1(a) the two-band calculations show a strong deviation from the lowest-order PT results. Note that Figs. 1(b), 1(c), and 1(d) are essentially the same except for a linear change in the vertical axis, as exciton shifts in the weak-field approximation are linear in the laser intensity. From this we may infer any result concerning the shifts in the weak-field limit, for this range of laser detuning. In Fig. 2 we show the exciton Stark shift as a function of the laser intensity, for different values of δ. It is also clear from Fig. 2(c) the increase in importance of considering a nonperturbative approach, if $\Lambda_0 \approx \delta$. In this situation it is again observed that there is a strong deviation from the lowest-order perturbation theory results. Figs. 1 and 2 clearly indicate the inadequacy of the HF Coulomb perturbative results in quantitatively describing situations of the real experiments (detunings of few tenths of meV) involving correlated $e-h$ pairs. We note that the Coulomb perturbative HF treatment is valid under the condition that $\Lambda_0 \ll \delta$ and $E_0 \ll \delta$, and that the convergence of the perturbative expansion on the Coulomb interaction is rather poor in the region of experimental interest (note that the Coulomb perturbative corrections may be larger than the $2\Lambda_0^2/\delta$ leading term).

As mentioned before, the above HF results are restricted to bulk systems, whereas many experimental situations are concerned with the observation of the optical Stark shifts of excitons in confined heterostructures such as QWs.[11,13,14] Of course, in this case a HF-type calculation is still more difficult due to the lack of exact exciton wave functions. On the other hand, it is straigthforward to use the renormalized mass dressed-band approach to perform the calculations for the exciton shifts[2–5] in any confined heterostructure for which the effective-mass approximation is valid.

The laser-induced changes in the GaAs gap and exciton binding energies in GaAs–(Ga,Al)As QWs lead to blueshifts in the exciton peak energies. The dressed-band calculation indicates that the most important contribution to the exciton blueshift originates from the laser effects on the GaAs gap, other contributions being the changes in the exciton binding energies and QW confinement both of free electrons and holes.[2–5] In this aspect, the importance of a realistic band-structure modeling may be inferred from the results shown in Fig. 3, where we display the shift of 1*s* exciton peak as a function of the laser intensity for both the two-band Calla-

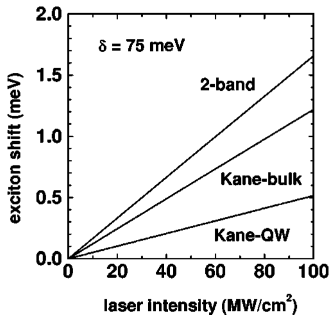

FIG. 3. Same as in Fig. 2 (δ=75 meV) including the results, within the laser-dressed Kane model, for both bulk GaAs and a 100 Å GaAs–$Ga_{0.7}Al_{0.3}As$ QW.

way and three-band Kane models[15,16] in bulk systems and the three-band Kane calculations[4] for a 100 Å GaAs–(Ga,Al)As QW, with a fixed detuning $\delta = 75$ meV. One notices that in the linear-intensity regime, the laser-dressed Kane model leads, in the lowest order, to an exciton blueshift given by $4\Lambda_0^2/3\delta$, whereas the two-band model results in a larger shift of $2\Lambda_0^2/\delta$, which corresponds to the zeroth-order term of the two-band HF diagrammatic approach. Besides the importance of a realistic band modeling, it is also clear from Fig. 3 that the quantum-well confinement plays a fundamental role in the exciton Stark shift. In this sense it is interesting to compare the theoretical results with experimental measurements concerning the 1s-like Stark shift in GaAs–(Ga,Al)As QWs. The measurements of von Lehmen *et al.*,[11] for a QW of width $\approx$100 Å, laser intensities of 10^4–10^6 W/cm^2, and detuning of 25 meV, leads to a Stark shift of 0.22 meV. In contrast, Joffre *et al.*[14] report essentially the same shift for a detuning of $\approx$65 meV and a QW of the same width, but for laser intensities at least 100 times larger, i.e., 10^8 W/cm^2. The present dressed-band results within the Kane–QW model (cf. Fig. 3), for the 100 Å GaAs–(Ga,Al)As QW and laser detuning of 75 meV, gives a shift of $\approx$0.5 meV if the laser intensity is $\approx 10^8$ W/cm^2, in fairly good agreement with the measurements by Joffre *et al.*[14] In the pioneering experiment of Mysyrowicz *et al.*,[13] the laser intensity was higher than 10^9 W/cm^2, for a GaAs–(Ga,Al)As QW of width $\approx$100 Å. We may estimate from their Fig. 1 the laser detuning to be $\approx$25 meV and the shift of the 1s exciton peak $\approx$2 meV. Of course, for this intensity and detuning regime, the perturbative limit is no longer valid [cf. Fig. 1(a)] and the nonperturbative dressed-band Kane–QW calculation, with a detuning of 25 meV, gives an exciton Stark shift of $\approx$10 meV, for 10^9 W/cm^2, which is in qualitative agreement with experiment.[13]

IV. CONCLUSIONS

In the present work, we have focused our attention in the well studied optical Stark shift of the 1s-like exciton peak in bulk and QW semiconductor systems. In the large detuning regime, it is well known that the Coulomb corrections to the exciton-peak shift may be treated as a perturbation to the one-body approximation. The simplest approach to introduce these corrections is the HF approximation. As shown, even in the laser field-perturbative regime, it has severe limitations. First, its convergence, even in the large detuning limit, is extremely slow. This is a strong restriction on the application of the field-perturbative HF scheme to real experimental situations, as discussed above. Second, it is certainly not trivial to extend this type of HF calculations to treat band-structure effects (beyond the two-band approximation) and appropriately account for the electron/hole confinement in heterostructure systems, such as the discussed GaAs–(Ga,Al)As QW. Finally, a comparison between experiments and the present three-band Kane-dressed GaAs–(Ga,Al)As QW results indicates, for a large range of detunings and laser intensities, the importance of a proper treatment of band-structure and QW-confinement effects in a quantitative understanding of Stark shift experimental measurements. In this sense, the renormalized dressed-band approach is a very convenient tool to treat, in the large detuning limit, processes involving the laser–semiconductor interaction in low-dimensional heterostructures.

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APPENDIX A

The weak-field limit of the exciton Stark shift

$$\Sigma_{\lambda\lambda} = \Pi_{\lambda\lambda} + \Delta_{\lambda\lambda}, \tag{A1}$$

associated to the $\lambda-$th exciton state $\phi_{\lambda\mathbf{k}}$, consists of two parts

$$\Pi_{\lambda\lambda} = 2\Lambda_0 \sum_{\mathbf{k}} |\phi_{\lambda\mathbf{k}}|^2 P_{\mathbf{k}}^*, \tag{A2}$$

and

$$\Delta_{\lambda\lambda} = 2\sum_{\mathbf{k},\mathbf{k}'} (\phi_{\lambda\mathbf{k}}^* - \phi_{\lambda\mathbf{k}'}^*)\phi_{\lambda\mathbf{k}'} V_{\mathbf{k}-\mathbf{k}'} P_{\mathbf{k}} (P_{\mathbf{k}}^* - P_{\mathbf{k}'}^*), \tag{A3}$$

which correspond to Eqs. (5) and (6) of Ell *et al.*,[7] and to Eqs. (16.14)–(16.16) of Haug and Koch.[8] Furthermore, as discussed by Combescot,[9] the derivation of Schmitt-Rink *et al.*[6] leads basically to the same equations. The Rabi energy is $\Lambda_0 = d_{cv}E_p$, with d_{cv} being the interband dipole matrix elements[1] and $E_p e^{-i\omega t}$+c.c. the monochromatic laser field,

$$P_{\mathbf{k}} = \Lambda_0 G_{\mathbf{k}} = \Lambda_{\mathbf{k}}/\delta_{\mathbf{k}} \tag{A4}$$

is the light-induced $e-h$ pair amplitude

$$\Lambda_{\mathbf{k}} = \Lambda_0 + \sum_{\mathbf{k}'} V_{\mathbf{k}-\mathbf{k}'} P_{\mathbf{k}'}, \tag{A5}$$

with $V_{\mathbf{k}-\mathbf{k}'} = 4\pi e^2/|\mathbf{k}-\mathbf{k}'|^2$ being the Coulomb interaction and

$$\delta_{\mathbf{k}} = \delta + \frac{\hbar^2 k^2}{2\mu^*}, \tag{A6}$$

where μ^* is the exciton reduced mass. One should note that the above equations are only correct in the weak-field limit

($\Lambda_0 \ll \delta$) and valid to $O(\Lambda_0^2/\delta)$. In order to have the laser tuned far below any exciton resonances, one should also have $E_0 \ll \delta$.

Equations (A1)–(A6) should be solved iteratively and we take

$$P_{\mathbf{k}} \approx P_{\mathbf{k}}^{(1)} = P_{\mathbf{k}}^{(0)} + G_{\mathbf{k}}^0 \sum_{\mathbf{k}'} V_{\mathbf{k}-\mathbf{k}'} P_{\mathbf{k}'}^{(0)} \quad \text{(A7)}$$

with

$$P_{\mathbf{k}}^{(0)} = \frac{\Lambda_0}{\delta_{\mathbf{k}}} = \Lambda_0 G_{\mathbf{k}}^0, \quad \text{(A8)}$$

in Eq. (A3), and

$$P_{\mathbf{k}} \approx P_{\mathbf{k}}^{(2)} = P_{\mathbf{k}}^{(0)} + G_{\mathbf{k}}^0 \sum_{\mathbf{k}'} V_{\mathbf{k}-\mathbf{k}'} P_{\mathbf{k}'}^{(0)} + G_{\mathbf{k}}^0 \sum_{\mathbf{k}',\mathbf{k}''} V_{\mathbf{k}-\mathbf{k}'} G_{\mathbf{k}'}^0 V_{\mathbf{k}'-\mathbf{k}''} P_{\mathbf{k}''}^{(0)} \quad \text{(A9)}$$

in Eq. (A2), so that both contributions are evaluated in the same order in the Coulomb interaction, i.e., $O(V^3)$. This leads to

$$\Pi_{\lambda\lambda} = 2\Lambda_0^2 \sum_{\mathbf{k}} |\phi_{\lambda\mathbf{k}}|^2 G_{\mathbf{k}} = 2\Lambda_0^2 \sum_{\mathbf{k}} |\phi_{\lambda\mathbf{k}}|^2 \left(G_{\mathbf{k}}^0 + \sum_{\mathbf{q}} G_{\mathbf{k}}^0 V_{\mathbf{q}} G_{\mathbf{k}+\mathbf{q}}^0 + \sum_{\mathbf{q},\mathbf{q}'} G_{\mathbf{k}}^0 V_{\mathbf{q}} G_{\mathbf{k}+\mathbf{q}}^0 V_{\mathbf{q}'} G_{\mathbf{k}+\mathbf{q}+\mathbf{q}'}^0 \right) + O(V^3), \quad \text{(A10)}$$

which is related to the $\tilde{\alpha}_i$ contribution to the exciton shift in the perturbation approach by Combescot[9] [see Eqs. (6.9)–(6.19) of Ref. 9]. Also, it is straightforward to show that

$$\Delta_{\lambda\lambda} = 2\Lambda_0^2 \sum_{\mathbf{k},\mathbf{q}} V_{\mathbf{q}} \phi_{\lambda\mathbf{k}}^* (\phi_{\lambda\mathbf{k}} - \phi_{\lambda\mathbf{k}+\mathbf{q}}) G_{\mathbf{k}+\mathbf{q}} (G_{\mathbf{k}} - G_{\mathbf{k}+\mathbf{q}}) = 2\Lambda_0^2 \sum_{\mathbf{k},\mathbf{q}} V_{\mathbf{q}} \phi_{\lambda\mathbf{k}}^* (\phi_{\lambda\mathbf{k}} - \phi_{\lambda\mathbf{k}+\mathbf{q}}) \Bigg[G_{\mathbf{k}+\mathbf{q}}^0 (G_{\mathbf{k}}^0 - G_{\mathbf{k}+\mathbf{q}}^0) + \sum_{\mathbf{q}'} G_{\mathbf{k}+\mathbf{q}}^0 V_{\mathbf{q}'} G_{\mathbf{k}+\mathbf{q}+\mathbf{q}'}^0 (G_{\mathbf{k}}^0 - G_{\mathbf{k}+\mathbf{q}}^0) + G_{\mathbf{k}+\mathbf{q}}^0 \left(\sum_{\mathbf{q}'} G_{\mathbf{k}}^0 V_{\mathbf{q}'} G_{\mathbf{k}+\mathbf{q}'}^0 - \sum_{\mathbf{q}'} G_{\mathbf{k}+\mathbf{q}}^0 V_{\mathbf{q}'} G_{\mathbf{k}+\mathbf{q}+\mathbf{q}'}^0 \right) \Bigg] + O(V^3), \quad \text{(A11)}$$

corresponding to the β_i contribution by Combescot[9] [see Eq. (6.30) of Ref. 9].

APPENDIX B

In order to obtain the shift of the 1s exciton peak, one uses

$$\phi_{\lambda\mathbf{k}} = \phi_{1s,\mathbf{k}} = \frac{8\sqrt{\pi a_0^3}}{[1+(ka_0)^2]^2}, \quad \text{(B1)}$$

where a_0 is the exciton Bohr radius. The total Π_{1s} contribution to the 1s Stark shift of the exciton peak, evaluated up to second order in the Coulomb interaction, i.e., $O(V^3)$, is given by

$$\Pi_{1s} = \Pi_{1s}^{(0)} + \Pi_{1s}^{(1)} + \Pi_{1s}^{(2)}, \quad \text{(B2)}$$

where

$$\Pi_{1s}^{(0)} = 2\Lambda_0^2 \sum_{\mathbf{k}} |\phi_{1s,\mathbf{k}}|^2 G_{\mathbf{k}}^0 = \frac{2\Lambda_0^2}{\delta}\left[1 - \frac{E_0}{\delta} + \dots\right], \quad \text{(B3)}$$

$$\Pi_{1s}^{(1)} = 2\Lambda_0^2 \sum_{\mathbf{k}} |\phi_{1s,\mathbf{k}}|^2 \sum_{\mathbf{q}} G_{\mathbf{k}}^0 V_{\mathbf{q}} G_{\mathbf{k}+\mathbf{q}}^0 = \frac{2\Lambda_0^2}{\delta}\left[2\sqrt{\frac{E_0}{\delta}} + O\left(\left(\frac{E_0}{\delta}\right)^{3/2}\right)\right], \quad \text{(B4)}$$

$$\Pi_{1s}^{(2)} = 2\Lambda_0^2 \sum_{\mathbf{k}} |\phi_{1s,\mathbf{k}}|^2 \sum_{\mathbf{q},\mathbf{q}'} G_{\mathbf{k}}^0 V_{\mathbf{q}} G_{\mathbf{k}+\mathbf{q}}^0 V_{\mathbf{q}'} G_{\mathbf{k}+\mathbf{q}+\mathbf{q}'}^0 = \frac{2\Lambda_0^2}{\delta}\left[4 \ln 2 \frac{E_0}{\delta} + \dots\right], \quad \text{(B5)}$$

whereas the Δ_{1s} contribution, to second order in the Coulomb interaction, is

$$\Delta_{1s} = \sum_{i=1,7} \Delta_{1s}^{(i)}, \quad \text{(B6)}$$

with

$$\Delta_{1s}^{(1)} = 2\Lambda_0^2 \sum_{\mathbf{k},\mathbf{q}} V_{\mathbf{q}} |\phi_{1s,\mathbf{k}}|^2 G_{\mathbf{k}+\mathbf{q}}^0 G_{\mathbf{k}}^0 = \frac{2\Lambda_0^2}{\delta}\left[2\sqrt{\frac{E_0}{\delta}} + O\left(\left(\frac{E_0}{\delta}\right)^{3/2}\right)\right], \quad \text{(B7)}$$

$$\Delta_{1s}^{(2)} = -2\Lambda_0^2 \sum_{\mathbf{k},\mathbf{q}} V_{\mathbf{q}} |\phi_{1s,\mathbf{k}}|^2 G_{\mathbf{k}+\mathbf{q}}^0 G_{\mathbf{k}+\mathbf{q}}^0 = \frac{2\Lambda_0^2}{\delta}\left[-\sqrt{\frac{E_0}{\delta}} + \dots\right], \quad \text{(B8)}$$

$$\Delta_{1s}^{(3)}=-2\Lambda_0^2\sum_{\mathbf{k},\mathbf{q}} V_{\mathbf{q}}\phi_{1s,\mathbf{k}}^*\phi_{1s,\mathbf{k}+\mathbf{q}}G_{\mathbf{k}+\mathbf{q}}^0G_{\mathbf{k}}^0 = -\frac{2\Lambda_0^2}{\delta}\left[2\frac{E_0}{\delta}+\dots\right], \tag{B9}$$

$$\Delta_{1s}^{(4)}=2\Lambda_0^2\sum_{\mathbf{k},\mathbf{q}} V_{\mathbf{q}}\phi_{1s,\mathbf{k}}^*\phi_{1s,\mathbf{k}+\mathbf{q}}G_{\mathbf{k}+\mathbf{q}}^0G_{\mathbf{k}+\mathbf{q}}^0 = \frac{2\Lambda_0^2}{\delta}\left[2\frac{E_0}{\delta}+\dots\right], \tag{B10}$$

$$\Delta_{1s}^{(5)}=2\Lambda_0^2\sum_{\mathbf{k},\mathbf{q}} V_{\mathbf{q}}\phi_{1s,\mathbf{k}}^*(\phi_{1s,\mathbf{k}}-\phi_{1s,\mathbf{k}+\mathbf{q}})G_{\mathbf{k}}^0G_{\mathbf{k}+\mathbf{q}}^0 \times\sum_{\mathbf{q}'} V_{\mathbf{q}'}G_{\mathbf{k}+\mathbf{q}+\mathbf{q}'}^0=\frac{2\Lambda_0^2}{\delta}\left[4\ln 2\frac{E_0}{\delta}+\dots\right], \tag{B11}$$

$$\Delta_{1s}^{(6)}=-4\Lambda_0^2\sum_{\mathbf{k},\mathbf{q}} V_{\mathbf{q}}\phi_{1s,\mathbf{k}}^*(\phi_{1s,\mathbf{k}}-\phi_{1s,\mathbf{k}+\mathbf{q}})G_{\mathbf{k}+\mathbf{q}}^0G_{\mathbf{k}+\mathbf{q}}^0 \times\sum_{\mathbf{q}'} V_{\mathbf{q}'}G_{\mathbf{k}+\mathbf{q}+\mathbf{q}'}^0=-\frac{2\Lambda_0^2}{\delta}\left[8\ln 2\frac{E_0}{\delta}+\dots\right], \tag{B12}$$

$$\Delta_{1s}^{(7)}=2\Lambda_0^2\sum_{\mathbf{k},\mathbf{q}} V_{\mathbf{q}}\phi_{1s,\mathbf{k}}^*(\phi_{1s,\mathbf{k}}-\phi_{1s,\mathbf{k}+\mathbf{q}})G_{\mathbf{k}}^0G_{\mathbf{k}+\mathbf{q}}^0 \times\sum_{\mathbf{q}'} V_{\mathbf{q}'}G_{\mathbf{k}+\mathbf{q}'}^0=\frac{2\Lambda_0^2}{\delta}\left[4\frac{E_0}{\delta}+\dots\right], \tag{B13}$$

where we have used the following relations:

$$\sum_{\mathbf{q}} V_{\mathbf{q}}G_{\mathbf{k}+\mathbf{q}}^0=H(k)=\frac{2\beta}{k}\tan^{-1}(k/\alpha), \tag{B14}$$

with $\beta=1/a_0$, $\alpha^2=2\mu^*\delta/\hbar^2$ (note that $\beta/\alpha=\sqrt{E_0/\delta}$),

$$J_n(\alpha,\beta)=\int_{-\infty}^{+\infty}\frac{k\,dk}{(k^2+\alpha^2)(k^2+\beta^2)^n}\tan^{-1}(k/\alpha),$$
$$J_1(\alpha,\beta)=-\frac{\pi}{\alpha^2-\beta^2}\ln\left(\frac{1+\beta/\alpha}{2}\right), \tag{B15}$$

with $J_n(\alpha,\beta)$ easily obtained from the above $n=1$ result, and

$$\sum_{\mathbf{q}} V_{\mathbf{q}}G_{\mathbf{k}+\mathbf{q}}^0|\phi_{1s,\mathbf{k}+\mathbf{q}}|^2=\left(\frac{64}{\pi}\right)\alpha^2\beta^4T_4(\alpha,\beta,k)\left(\frac{E_0}{\delta}\right),$$

$$T_n(\alpha,\beta,k) =2\pi\int_{-1}^{+1}du\int_0^{\infty} \times\frac{dq}{(k^2+q^2+2kqu+\alpha^2)(k^2+q^2+2kqu+\beta^2)^n}, \tag{B16}$$

$$T_1(\alpha,\beta,k)=\frac{2\pi^2}{k(\alpha^2-\beta^2)}[\tan^{-1}(k/\beta)-\tan^{-1}(k/\alpha)]. \tag{B17}$$

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