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Optical properties of quantum wires: Disorder scattering in the Lloyd model

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The Lloyd model is extended to the exciton problem in quasi-one-dimensional structures to study the interplay between the Coulomb attraction and disorder scattering. Within this model the averaging and resummation of the locator series can be performed analytically. As an application, the optical absorption in quantum box wires is investigated. Without electron–hole interaction, fluctuations in the well width lead to an asymmetric broadening of the minibands with respect to the lower and upper band edges.

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I. INTRODUCTION

The optical properties of semiconductors near the band edge are substantially influenced by the attractive electron–hole interaction which leads to pronounced excitonic lines and enhanced absorption above the band gap.[1] These phenomena become even more pronounced in systems of reduced effective dimensionality such as quantum wells, wires, or dots. In addition, the influence of disorder and impurity scattering increases with decreasing dimension. The latter phenomenon, however, is usually considered phenomenologically by replacing the light frequency ω by $\omega+i\gamma$, or convoluting the spectrum with an appropriate smoothing function of width γ.

In this article, we investigate the interplay between excitonic effects and disorder scattering in quasi-one-dimensional structures, in particular quantum wires which possess a periodic step-like modulation along the one-dimensional direction, [quantum box structures, (QBS)] Fig. 1. Such structures have been proposed as favorite candidates to generate Bloch oscillations,[2–4] other examples are quasi-one-dimensional molecular crystals,[5–9] yet no detailed theoretical study of the optical properties has been published. The optical properties of one-dimensional systems are exceptional as even a small attractive electron–hole interaction leads to a drastic reduction in the oscillator strength at the gap energy so that the identification of the gap energy from optical absorption data is nontrivial.

Our paper is organized as follows: Section II summarizes the basic description of the optical susceptibility in terms of the resolvent operator. In Secs. III and IV the averaging on the disordered chain is performed. Within a Wannier representation the averaging and resummation of the locator expansion can be done exactly, provided (a) only the lowest electron/hole subbands are considered, and (b) a Lorentzian probability distribution for the disorder averaging is used. The latter is known as the Lloyd model,[10] which has been first used in connection with the calculation of the density of states in a disordered metal and due to the simplicity in calculating various averages this model has been found useful by many other researchers, in particular Refs. 11–25. However, apart from Hoshino's work[13] on the electrical conductivity (CPA, neglecting vertex corrections) all previous applications of the Lloyd model are exclusively restricted to single-particle quantities. Our work extends the Lloyd model to a two-particle quantity and we give an exact solution for the optical absorption within a two-band model. Section V gives some analytical and numerical results for QBS's near the fundamental gap and Sec. VI contains our conclusions.

II. BASICS

Our starting point is the excitonic contribution to the optical susceptibility $\chi(\omega)$ in a two-band effective mass approximation[1,26]

$$\chi(\omega)=-\frac{2|d\mathrm{cv}|^2}{\epsilon_0\Omega}\sum_n\frac{1}{\hbar\omega+\imath\delta-E_n}\left|\int_\Omega d^3\vec{r}\,\Psi_n(\vec{r},\vec{r})\right|^2, \tag{1}$$

where the nonresonant part has been neglected $(\omega>0)$. Ω is the volume of the sample, and $|d_{\mathrm{cv}}|^2$ is the dipole matrix element between the valence and conduction band. $\Psi_n(\vec{r}_e,\vec{r}_h)$, E_n, respectively, denote the electron–hole envelope function and energy, and n labels discrete as well as the continuous part of the excitonic spectrum,

$$[H_{\mathrm{e}}+H_{\mathrm{h}}+V(\vec{r}_{\mathrm{e}}-\vec{r}_{\mathrm{h}})]\Psi_n(\vec{r}_{\mathrm{e}},\vec{r}_{\mathrm{h}})=E_n\Psi_n(\vec{r}_{\mathrm{e}},\vec{r}_{\mathrm{h}}). \tag{2}$$

H_j, $j=e,h$ denote the electron/hole Hamiltonians and $V(\vec{r})$ is the attractive electron–hole Coulomb potential. We assume a cylindrical wire of radius R with an infinite confining potential and restrict ourselves to the lowest electron/hole mini-bands with wave functions $\Psi_j(\vec{r})=u(r_\perp)\psi_j(z)$. $u(r_\perp)$ is radial symmetric, nodeless and $\psi_j(z)$ denote the wave function along the wire z axis which obeys

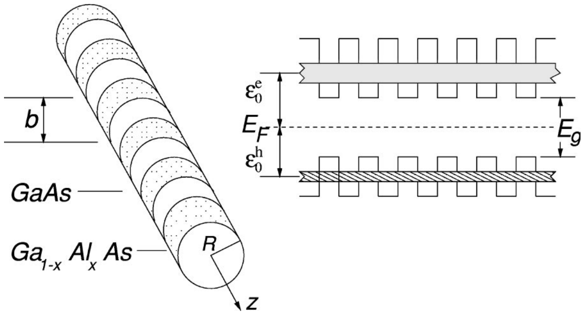

FIG. 1. Quasi-one-dimensional quantum-box-structure (left) and sketch of the lowest valence/conduction subbands (right). (Not to scale.)

$$H_j \psi_j(z) = E_j \psi_j(z), \tag{3}$$

$$H_j = \frac{-\hbar^2}{2m_j} \frac{\partial^2}{\partial z^2} + V_j(z). \tag{4}$$

m_j are the effective electron/hole masses and $V_j(z)$ includes the band offset as well as the localization energy due to the radial confinement. For a homogeneous wire the energy spectrum consists of free-electron-like mini-bands with parabolic dispersions. These bands will be additionally split into subbands by the periodic modulation in composition along the wire axis. In the following we restrict ourselves to the lowest electron and hole subbands which are conveniently described in terms of Wannier functions $a_j(z-pb)$, where p labels sites and b is the period of the box structure, see Fig. 1. By an appropriate choice of the phases of the Bloch functions $\psi_j(k,z)$ the Wannier functions can be constructed in such a way that they are real, symmetric, and exponentially localized.[27] Furthermore, the Wannier functions of the lowest hole and electron subbands both have the same even parity,

$$\Psi_n(z_e, z_h) = \sum_{p_e, p_h} \psi^{(n)}_{p_e, p_h} a_e(z_e - p_e b) a_h(z_h - p_h b), \tag{5}$$

$$\sum_{\bar{p}_e, \bar{p}_h} \mathcal{H}_{p_e p_h \bar{p}_e \bar{p}_h} \psi^{(n)}_{\bar{p}_e \bar{p}_h} = E_n \psi^{(n)}_{p_e p_h}. \tag{6}$$

Within a next neighbor approximation the matrix elements of the exciton Hamiltonian $\boldsymbol{\mathcal{H}} = \boldsymbol{\mathcal{H}}^e + \boldsymbol{\mathcal{H}}^h + \boldsymbol{\mathcal{V}}$ read

$$\mathcal{H}_{p_e p_h \bar{p}_e \bar{p}_h} = \delta_{p_h \bar{p}_h} \mathcal{H}^e_{p_e \bar{p}_e} + \delta_{p_e \bar{p}_e} \mathcal{H}^h_{p_h \bar{p}_h} + \mathcal{V}_{p_e p_h \bar{p}_e \bar{p}_h}, \tag{7}$$

$$\mathcal{H}^{(j)}_{p,\bar{p}} = \mathcal{D}^{(j)}_{p,\bar{p}} + \mathcal{N}^{(j)}_{p,\bar{p}}, \tag{8}$$

$$\mathcal{D}^{(j)}_{p,\bar{p}} = \delta_{p,\bar{p}} \epsilon^{(j)}_0, \tag{9}$$

$$\mathcal{N}^{(j)}_{p,\bar{p}} = t^{(j)}_1 \{ \delta_{\bar{p},p+1} + \delta_{p,\bar{p}+1} \}. \tag{10}$$

$\epsilon^{(j)}_0, t^{(j)}_1$, respectively, denote the on-site energies and transfer elements between neighboring wells and $\mathcal{V}_{p_e p_h \bar{p}_e \bar{p}_h} \approx V(p_e - p_h) \delta_{p_e \bar{p}_e} \delta_{p_h \bar{p}_h}$ is the electron–hole Coulomb matrix element.

To calculate the optical absorption we rewrite Eq. (1) in terms of the resolvent operator $\mathcal{G}(\tilde{E})$,

$$\chi(\hbar\omega) \propto -\sum_{p,\bar{p}} \mathcal{G}_{p,p,\bar{p},\bar{p}}(\hbar\omega + \imath\delta), \tag{11}$$

$$\boldsymbol{\mathcal{G}}(\tilde{E}) = (\tilde{E} - \boldsymbol{\mathcal{H}})^{-1}, \tag{12}$$

where $\tilde{E} = E + \imath\delta$, $\delta > 0$.

Without disorder, the electron-hole wave function obeys the Bloch theorem and, hence, it can be labeled by a wave number $k = 2\pi\kappa/N$, $\kappa = 0, \pm 1, \ldots \pm N/2$,

$$\psi^{(n,k)}_{p_e+\nu, p_h+\nu} = e^{\imath k b \nu} \psi^{(n,k)}_{p_e, p_h}. \tag{13}$$

$\nu = 1,2 \ldots N$, where N is the number of sites on the chain. Periodic boundary conditions are implied. Hence,

$$\mathcal{G}_{p_e, p_h, \bar{p}_e, \bar{p}_h}(\tilde{E}) = \sum_{n,k} \frac{\psi^{*(n,k)}_{p_e, p_h} \psi^{(n,k)}_{\bar{p}_e, \bar{p}_h}}{\tilde{E} - E_{n,k}}$$

$$= \mathcal{G}_{p_e+\nu, p_h+\nu, \bar{p}_e+\nu, \bar{p}_h+\nu}(\tilde{E}). \tag{14}$$

Furthermore, only $k=0$ states $\psi^{(n,k=0)}_{p_e,p_h} = \phi^{(n)}_{p_e - p_h}$ contribute to the optical absorption

$$\sum_{p,\bar{p}} \mathcal{G}_{p,p,\bar{p},\bar{p}}(\tilde{E}) = N \sum_{p} \mathcal{G}_{p,p,0,0}(\tilde{E}) = N \sum_{n} \frac{\phi^{*(n)}_0 \phi^{(n)}_0}{\tilde{E} - E_n}$$

$$= N G_{00}(\tilde{E}). \tag{15}$$

The $k=0$ states are translational invariant and effectively describe a single particle in an external potential

$$(t^h_1 + t^e_1)(\phi^{(n)}_{r+1} + \phi^{(n)}_{r-1}) + (\epsilon^h_0 + \epsilon^e_0)\phi^{(n)}_r + V_r \phi^{(n)}_r = E_n \phi^{(n)}_r,$$

$$r \in \mathcal{Z}. \tag{16}$$

$G_{r,\bar{r}}(\tilde{E})$ is the corresponding Green function which obeys the Dyson equation

$$\mathbf{G} = \mathbf{G}_0 + \mathbf{G}_0 \mathbf{V} \mathbf{G}. \tag{17}$$

Boldface symbols denote matrices, $\mathbf{G}_0$ is the Green function for $V_r = 0$, and $\mathbf{V}$ is a diagonal matrix, $V_{rr'} = V_r \delta_{rr'}$. The formal solution of Eq. (17) is obtained by matrix inversion

$$\mathbf{G} = (\mathbf{1} - \mathbf{G}_0 \mathbf{V})^{-1} \mathbf{G}_0. \tag{18}$$

In addition to the attractive electron–hole interaction we shall consider fluctuations in the on-site energies ϵ_0 as well as in the transfer elements t_1 between adjacent wells of the Kronig–Penny potential. Such fluctuations arise from compositional and structural disorder of the wire and we assume that these fluctuations preserve the radial symmetry so that mixing of higher subbands will not be important.

III. BARRIER FLUCTUATIONS

Fluctuation in the barrier thickness leads to coupled fluctuations in the on-site energies and the transfer elements between sites q and $q+1$ (nondiagonal disorder). In particular, we consider a correlated linear change of the on-site energies as mentioned by John and Schreiber.[12] For the lowest subband t_1 is negative, thus, corrections to the on-site energies and hopping element have the same sign, i.e., $\epsilon_q = \alpha \Delta t$, $\alpha > 0$. (The coupling of diagonal and nondiagonal disorder will be essential to guarantee the convergence of the locator expansion and nonnegative absorption.) For simplicity, fluctuations in the electron and hole parameters are assumed to be independent so that the Hamiltonians Eq. (7) are replaced by

$$\mathcal{D}^{(j)}_{p,\bar{p}} = \epsilon^{(j)}_0 + \alpha^{(j)} \Delta t^{(j)}_{p,p+1} + \alpha^{(j)} \Delta t^{(j)}_{p,p-1}, \tag{19}$$

$$\mathcal{N}^{(j)}_{p,\bar{p}}=\delta_{\bar{p},p+1}\{t_1^{(j)}+\Delta t^{(j)}_{\bar{p},p+1}\}+\delta_{p,\bar{p}+1}\{t_1^{(j)}+\Delta t^{(j)}_{p,\bar{p}+1}\}. \tag{20}$$

In matrix notation $\boldsymbol{\mathcal{H}}=\boldsymbol{\mathcal{D}}+\boldsymbol{\mathcal{N}}+\boldsymbol{\mathcal{V}}$, where $\boldsymbol{\mathcal{D}},\boldsymbol{\mathcal{N}}$ include electron and hole parts. To perform the disorder averaging the locator expansion of the resolvent will be used[28]

$$\boldsymbol{\mathcal{G}}(\tilde{E})=\sum_{n=0}^{\infty}\boldsymbol{\mathcal{G}}^{(n)}(\tilde{E}), \tag{21}$$

$$\boldsymbol{\mathcal{G}}^{(n)}(\tilde{E})=\frac{1}{\tilde{E}-\boldsymbol{\mathcal{D}}}\left[\boldsymbol{\mathcal{M}}\frac{1}{\tilde{E}-\boldsymbol{\mathcal{D}}}\right]^{n}, \tag{22}$$

where $\boldsymbol{\mathcal{M}}=\boldsymbol{\mathcal{N}}+\boldsymbol{\mathcal{V}}$. As $\boldsymbol{\mathcal{D}}$ is a diagonal matrix, we have $(n\geqslant 2)$

$$\mathcal{G}^{(0)}_{p_\mathrm{e}p_\mathrm{h}\bar{p}_\mathrm{e}\bar{p}_\mathrm{h}}(\tilde{E})=\frac{\delta_{p_\mathrm{e}p_\mathrm{e}}\delta\overline{p}_\mathrm{h}\overline{p}_\mathrm{h}}{\tilde{E}-\mathcal{D}_{p_\mathrm{e}p_\mathrm{h}p_\mathrm{e}p_\mathrm{h}}}, \tag{23}$$

$$\mathcal{G}^{(1)}_{p_\mathrm{e}p_\mathrm{h}\bar{p}_\mathrm{e}\bar{p}_\mathrm{h}}(\tilde{E})=\frac{1}{\tilde{E}-\mathcal{D}_{p_\mathrm{e}p_\mathrm{h}p_\mathrm{e}p_\mathrm{h}}}\,\frac{\mathcal{M}_{p_\mathrm{e}p_\mathrm{h}\bar{p}_\mathrm{e}\bar{p}_\mathrm{h}}}{\tilde{E}-\mathcal{D}_{\bar{p}_\mathrm{e}\bar{p}_\mathrm{h}\bar{p}_\mathrm{e}\bar{p}_\mathrm{h}}}, \tag{24}$$

$$\begin{aligned}\mathcal{G}^{(n)}_{p_\mathrm{e}p_\mathrm{h}\bar{p}_\mathrm{e}\bar{p}_\mathrm{h}}(\tilde{E})=&\sum_{p_\mathrm{e}^1p_\mathrm{h}^1}\cdots\sum_{p_\mathrm{e}^{(n-1)}p_\mathrm{h}^{(n-1)}}\frac{1}{\tilde{E}-\mathcal{D}_{p_\mathrm{e}p_\mathrm{h}p_\mathrm{e}p_\mathrm{h}}}\\&\times\frac{\mathcal{M}_{p_\mathrm{e}p_\mathrm{h}p_\mathrm{e}^{(1)}p_\mathrm{h}^{(1)}}}{\tilde{E}-\mathcal{D}_{p_\mathrm{e}^{(1)}p_\mathrm{h}^{(1)}p_\mathrm{e}^{(1)}p_\mathrm{h}^{(1)}}}\,\frac{\mathcal{M}_{p_\mathrm{e}^{(1)}p_\mathrm{h}^{(1)}p_\mathrm{e}^{(2)}p_\mathrm{h}^{(2)}}}{\tilde{E}-\mathcal{D}_{p_\mathrm{e}^{(2)}p_\mathrm{h}^{(2)}p_\mathrm{e}^{(2)}p_\mathrm{h}^{(2)}}}\cdots\\&\times\frac{\mathcal{M}_{p_\mathrm{e}^{(n-2)}p_\mathrm{h}^{(n-2)}p_\mathrm{e}^{(n-1)}p_\mathrm{h}^{(n-1)}}}{\tilde{E}-\mathcal{D}_{p_\mathrm{e}^{(n-1)}p_\mathrm{h}^{(n-1)}p_\mathrm{e}^{(n-1)}p_\mathrm{h}^{(n-1)}}}\\&\times\frac{\mathcal{M}_{p_\mathrm{e}^{(n-1)}p_\mathrm{h}^{(n-1)}\bar{p}_\mathrm{e}\bar{p}_\mathrm{h}}}{\tilde{E}-\mathcal{D}_{\bar{p}_\mathrm{e}\bar{p}_\mathrm{h}\bar{p}_\mathrm{e}\bar{p}_\mathrm{h}}}.\end{aligned} \tag{25}$$

Next, the disorder averaging will be performed term by term. Concerning the factors

$$\frac{\mathcal{M}_{p_\mathrm{e}p_\mathrm{h}\bar{p}_\mathrm{e}\bar{p}_\mathrm{h}}}{\tilde{E}-\mathcal{D}_{\bar{p}_\mathrm{e}\bar{p}_\mathrm{h}\bar{p}_\mathrm{e}\bar{p}_\mathrm{h}}} \tag{26}$$

four cases must be distinguished.

(1) $(p_\mathrm{e}=\overline{p}_\mathrm{e},\ p_\mathrm{h}=\overline{p}_\mathrm{h})$:

$$\frac{\mathcal{M}_{p_\mathrm{e}p_\mathrm{h}\bar{p}_\mathrm{e}\bar{p}_\mathrm{h}}}{\tilde{E}-\mathcal{D}_{\bar{p}_\mathrm{e}\bar{p}_\mathrm{h}\bar{p}_\mathrm{e}\bar{p}_\mathrm{h}}}=\frac{\mathcal{V}_{\bar{p}_\mathrm{e}\bar{p}_\mathrm{h}\bar{p}_\mathrm{e}\bar{p}_\mathrm{h}}}{\tilde{E}-\epsilon_0^\mathrm{e}-\epsilon_0^\mathrm{h}-\alpha^\mathrm{e}\{\Delta t^\mathrm{e}_{\bar{p}_\mathrm{e},\bar{p}_\mathrm{e}+1}+\Delta t^\mathrm{e}_{\bar{p}_\mathrm{e}-1,\bar{p}_\mathrm{e}}\}-\alpha^\mathrm{h}\{\Delta t^\mathrm{h}_{\bar{p}_\mathrm{h},\bar{p}_\mathrm{h}+1}+\Delta t^\mathrm{h}_{\bar{p}_\mathrm{h}-1,\bar{p}_\mathrm{h}}\}}. \tag{27}$$

(2) $(p_\mathrm{e}=\overline{p}_\mathrm{e},\ p_\mathrm{h}\neq\overline{p}_\mathrm{h})$

$$\frac{\mathcal{M}_{p_\mathrm{e}p_\mathrm{h}\bar{p}_\mathrm{e}\bar{p}_\mathrm{h}}}{\tilde{E}-\mathcal{D}_{\bar{p}_\mathrm{e}\bar{p}_\mathrm{h}\bar{p}_\mathrm{e}\bar{p}_\mathrm{h}}}=\frac{\mathcal{V}_{p_\mathrm{e}p_\mathrm{h}p_\mathrm{e}\bar{p}_\mathrm{h}}+\delta_{\bar{p}_\mathrm{h},p_\mathrm{h}+1}\{t_1^\mathrm{h}+\Delta t^\mathrm{h}_{p_\mathrm{h},p_\mathrm{h}+1}\}+\delta_{p_\mathrm{h},\bar{p}_\mathrm{h}+1}\{t_1^\mathrm{h}+\Delta t^\mathrm{h}_{\bar{p}_\mathrm{h},\bar{p}_\mathrm{h}+1}\}}{\tilde{E}-\epsilon_0^\mathrm{e}-\epsilon_0^\mathrm{h}-\alpha^\mathrm{e}\{\Delta t^\mathrm{e}_{\bar{p}_\mathrm{e},\bar{p}_\mathrm{e}+1}+\Delta t^\mathrm{e}_{\bar{p}_\mathrm{e}-1,\bar{p}_\mathrm{e}}\}-\alpha^\mathrm{h}\{\Delta t^\mathrm{h}_{\bar{p}_\mathrm{h},\bar{p}_\mathrm{h}+1}+\Delta t^\mathrm{h}_{\bar{p}_\mathrm{h}-1,\bar{p}_\mathrm{h}}\}}. \tag{28}$$

(3) $(p_\mathrm{e}\neq\overline{p}_\mathrm{e},\ p_\mathrm{h}=\overline{p}_\mathrm{h})$

$$\frac{\mathcal{M}_{p_\mathrm{e}p_\mathrm{h}\bar{p}_\mathrm{e}\bar{p}_\mathrm{h}}}{\tilde{E}-\mathcal{D}_{\bar{p}_\mathrm{e}\bar{p}_\mathrm{h}\bar{p}_\mathrm{e}\bar{p}_\mathrm{h}}}=\frac{\mathcal{V}_{p_\mathrm{e}p_\mathrm{h}\bar{p}_\mathrm{e}p_\mathrm{h}}+\delta_{\bar{p}_\mathrm{e},p_\mathrm{e}+1}\{t_1^\mathrm{e}+\Delta t^\mathrm{e}_{p_\mathrm{e},p_\mathrm{e}+1}\}+\delta_{p_\mathrm{e},\bar{p}_\mathrm{e}+1}\{t_1^\mathrm{e}+\Delta t^\mathrm{e}_{\bar{p}_\mathrm{e},\bar{p}_\mathrm{e}+1}\}}{\tilde{E}-\epsilon_0^\mathrm{e}-\epsilon_0^\mathrm{h}-\alpha^\mathrm{e}\{\Delta t^\mathrm{e}_{\bar{p}_\mathrm{e},\bar{p}_\mathrm{e}+1}+\Delta t^\mathrm{e}_{\bar{p}_\mathrm{e}-1,\bar{p}_\mathrm{e}}\}-\alpha^\mathrm{h}\{\Delta t^\mathrm{h}_{\bar{p}_\mathrm{h},\bar{p}_\mathrm{h}+1}+\Delta t^\mathrm{h}_{\bar{p}_\mathrm{h}-1,\bar{p}_\mathrm{h}}\}}. \tag{29}$$

(4) $(p_\mathrm{e}\neq\overline{p}_\mathrm{e},\ p_\mathrm{h}\neq\overline{p}_\mathrm{h})$ analogous to case (1).

The averaging procedure requires the evaluation of the following multiple integrals

$$\begin{aligned}\langle\mathcal{G}^{(n)}_{p_\mathrm{e}p_\mathrm{h}\bar{p}_\mathrm{e}\bar{p}_\mathrm{h}}(\tilde{E})\rangle=&\int_{-\infty}^{\infty}d\Delta t_{12}^\mathrm{e}\ldots d\Delta t_{N1}^\mathrm{e}d\Delta t_{12}^\mathrm{h}\ldots d\Delta t_{N1}^\mathrm{h}P\\&\times(\Delta t_{12}^\mathrm{e},\gamma^\mathrm{e})\ldots P(\Delta t_{N1}^\mathrm{e},\gamma^\mathrm{e})P\\&\times(\Delta t_{12}^\mathrm{h},\gamma^\mathrm{h})\ldots P(\Delta t_{N1}^\mathrm{h},\gamma^\mathrm{h})\mathcal{G}^{(n)}_{p_\mathrm{e}p_\mathrm{h}\bar{p}_\mathrm{e}\bar{p}_\mathrm{h}}\\&\times(\tilde{E},\Delta t_{12}^\mathrm{e},\ldots,\Delta t_{N1}^\mathrm{e},\Delta t_{12}^\mathrm{h},\ldots,\Delta t_{N1}^\mathrm{h}),\end{aligned} \tag{30}$$

where $P(\Delta,\gamma)$ is the probability distribution function on the disorder configurations. In the Lloyd model this function is a Lorentzian

$$P(\Delta,\gamma)=\frac{\gamma}{\pi}\,\frac{1}{\Delta^2+\gamma^2}, \tag{31}$$

where γ parametrizes the width of the distribution.

The integrations in Eq. (30) will be performed step by step in the indicated sequence. In Eqs. (23)–(25) each factor is a holomorphic function of Δt_{12}^h in the lower complex plane including the real axis, in addition, this function is bounded if $\alpha^{\mathrm{h}}\neq 0$. Thus, the averaging can be performed by contour integration closing the integration path in the lower $\Delta t_{12}^{\mathrm{h}}$ plane where Eq. (31) has a first-order pole. This just leads to a replacement of $\Delta t_{12}^{\mathrm{h}}$ by $-\imath\gamma^{\mathrm{h}}$. Further integrations follow the same reasoning. Hence, the resummation of the locator series is trivially possible and, as a result, we obtain

$$\bar{\boldsymbol{\mathcal{G}}}:=\langle\boldsymbol{\mathcal{G}}(\tilde{E})\rangle=(\tilde{E}-\bar{\boldsymbol{\mathcal{H}}})^{-1}. \tag{32}$$

$\boldsymbol{\mathcal{H}}$ is an effective Hamiltonian where the electron/hole parts of Eq. (7) are replaced by

$$\begin{aligned}\overline{\mathcal{H}}^{(j)}_{p,\bar{p}}=&\ \delta_{p,\bar{p}}(\epsilon_0^{(j)}-2\imath\gamma^{(j)}\alpha^{(j)})\\&+(\delta_{p,\bar{p}+1}+\delta_{\bar{p},p+1})(t_1^{(j)}-\imath\gamma^{(j)}).\end{aligned} \tag{33}$$

Thus, the influence of barrier disorder is captured by the resolvent of the pure wire where $\epsilon_0^{(j)},t_1^{(j)}$ are replaced by complex parameters $\overline{\epsilon_0^{(j)}}=\epsilon_0^{(j)}-2\imath\gamma^{(j)}\alpha^{(j)}$, $\overline{t_1^{(j)}}=t_1^{(j)}-\imath\gamma^{(j)}$. Although, Eq. (33) is no longer hermitian, eigenstates exist and, moreover, these are of the same form as for the pure wire, in particular the eigenvalues are

$$E^{(j)}(k)=\overline{\epsilon_0^{(j)}}+2\overline{t_1^{(j)}}\cos(kb). \tag{34}$$

For $t_1^{(j)}<0$ the lower/upper band edges are at $kb=0/\pi$ so that the complex electron/hole energies are distributed between $\epsilon_0-2|t_1|-2\imath\gamma(\alpha+1)$ and $\epsilon_0+2|t_1|-2\imath\gamma(\alpha-1)$. The parameter α must be restricted to $\alpha\geqslant 1$ for both electrons and holes, otherwise there will be energies with a positive imaginary part, i.e., the Green function will have poles in the upper energy plane which would violate causality. In addition, the optical absorption would become negative in some part of the spectrum. Note, that the correlated fluctuations in the diagonal/nondiagonal disorder will not simply lead to a Lorentzian smoothening of the absorption spectrum. In particular, for $\alpha=1$ the correlated shift of the on-site energies and transfer elements exactly cancel at the upper band edge so that the square root singularity of the density of states survives if electron–hole interaction is omitted.

IV. WELL FLUCTUATIONS

Fluctuations in the well sections predominantly lead to fluctuations in the on-site energies ϵ_q. For convenience, fluctuations in the hopping elements will be omitted, however, a correlation of the electron/hole energies will be retained: $\Delta_p^{\mathrm{h}}=\alpha\Delta_p^{\mathrm{e}}$, $\alpha\approx m_e/m_h>0$ (diagonal disorder).

To perform the disorder averaging a regrouping of the Hamitonian as $\boldsymbol{\mathcal{H}}=\boldsymbol{\mathcal{B}}+\boldsymbol{\mathcal{M}}$ is necessary, where

$$\begin{aligned}\mathcal{M}_{p_{\mathrm{e}}p_{\mathrm{h}}\bar{p}_{\mathrm{e}}\bar{p}_{\mathrm{h}}}=&\ \delta_{\bar{p}_{\mathrm{h}}p_{\mathrm{h}}}\{\delta_{\bar{p}_{\mathrm{e}}p_{\mathrm{e}}}\epsilon_0^{\mathrm{e}}+t_1^{\mathrm{e}}(\delta_{\bar{p}_{\mathrm{e}},p_{\mathrm{e}}+1}+\delta_{\bar{p}_{\mathrm{e}},p_{\mathrm{e}}-1})\}\\&+\delta_{\bar{p}_{\mathrm{e}}p_{\mathrm{e}}}\{\delta_{\bar{p}_{\mathrm{h}}p_{\mathrm{h}}}\epsilon_0^{\mathrm{h}}+t_1^{\mathrm{h}}(\delta_{\bar{p}_{\mathrm{h}},p_{\mathrm{h}}+1}+\delta_{\bar{p}_{\mathrm{h}},p_{\mathrm{h}}-1})\}\\&+\mathcal{V}_{p_{\mathrm{e}}p_{\mathrm{h}}\bar{p}_{\mathrm{e}}\bar{p}_{\mathrm{h}}},\end{aligned} \tag{35}$$

$$\mathcal{B}_{p_{\mathrm{e}}p_{\mathrm{h}}\bar{p}_{\mathrm{e}}\bar{p}_{\mathrm{h}}}=\delta_{\bar{p}_{\mathrm{h}}p_{\mathrm{h}}}\Delta^{\mathrm{h}}_{p_{\mathrm{h}}}+\delta_{\bar{p}_{\mathrm{e}}p_{\mathrm{e}}}\Delta^{\mathrm{e}}_{p_{\mathrm{e}}}. \tag{36}$$

Using the locator expansion Eqs. (21),(22) with $\boldsymbol{\mathcal{D}}$ replaced by $\boldsymbol{\mathcal{B}}$ the matrix elements of the resolvent become $(n\geqslant 2)$

$$\mathcal{G}^{(0)}_{p_{\mathrm{e}}\bar{p}_{\mathrm{e}}}\delta_{p_{\mathrm{h}}\bar{p}_{\mathrm{h}}}=\frac{\delta_{p_{\mathrm{e}}p_{\mathrm{h}}\bar{p}_{\mathrm{e}}\bar{p}_{\mathrm{h}}}}{\tilde{E}-(\Delta_{p_{\mathrm{e}}}+\alpha\Delta_{p_{\mathrm{h}}})}, \tag{37}$$

$$\mathcal{G}^{(1)}_{p_{\mathrm{e}}p_{\mathrm{h}}\bar{p}_{\mathrm{e}}\bar{p}_{\mathrm{h}}}=\frac{1}{\tilde{E}-(\Delta_{p_{\mathrm{e}}}+\alpha\Delta_{p_{\mathrm{h}}})}\,\frac{\mathcal{M}_{p_{\mathrm{e}}p_{\mathrm{h}}\bar{p}_{\mathrm{e}}\bar{p}_{\mathrm{h}}}}{\tilde{E}-(\Delta_{\bar{p}_{\mathrm{e}}}+\alpha\Delta_{\bar{p}_{\mathrm{h}}})}, \tag{38}$$

$$\begin{aligned}\mathcal{G}^{(n)}_{p^1_{\mathrm{e}},p^1_{\mathrm{h}},\bar{p}_{\mathrm{e}},\bar{p}_{\mathrm{h}}}=&\sum_{p^1_{\mathrm{e}},p^1_{\mathrm{h}}}\cdots\sum_{p^{n-1}_{\mathrm{e}},p^{n-1}_{\mathrm{h}}}\frac{1}{\tilde{E}-(\Delta_{p_{\mathrm{e}}}+\alpha\Delta_{p_{\mathrm{h}}})}\\&\times\frac{\mathcal{M}_{p_{\mathrm{e}}p_{\mathrm{h}}p^1_{\mathrm{e}}p^1_{\mathrm{h}}}}{\tilde{E}-(\Delta_{p^1_{\mathrm{e}}}+\alpha\Delta_{p^1_{\mathrm{h}}})}\,\frac{\mathcal{M}_{p^1_{\mathrm{e}}p^1_{\mathrm{h}}p^2_{\mathrm{e}}p^2_{\mathrm{h}}}}{\tilde{E}-(\Delta_{p^2_{\mathrm{e}}}+\alpha\Delta_{p^2_{\mathrm{h}}})}\cdots\\&\times\frac{\mathcal{M}_{p^{n-2}_{\mathrm{e}}p^{n-2}_{\mathrm{h}}p^{n-1}_{\mathrm{e}}p^{n-1}_{\mathrm{h}}}}{\tilde{E}-(\Delta_{p^{n-1}_{\mathrm{e}}}+\alpha\Delta_{p^{n-1}_{\mathrm{h}}})}\,\frac{\mathcal{M}_{p^{n-1}_{\mathrm{e}}p^{n-1}_{\mathrm{h}}\bar{p}_{\mathrm{e}}\bar{p}_{\mathrm{h}}}}{\tilde{E}-(\Delta_{\bar{p}_{\mathrm{e}}}+\alpha\Delta_{\bar{p}_{\mathrm{h}}})}.\end{aligned} \tag{39}$$

The disorder averaging of $\boldsymbol{\mathcal{G}}$ is done along the same route as before

$$\begin{aligned}\bar{\boldsymbol{\mathcal{G}}}:=&\int_{-\infty}^{\infty}d\Delta_1\cdots d\Delta_N P(\Delta_1,\gamma)\cdots P(\Delta_N,\gamma)\mathcal{G}^{(n)}_{p_{\mathrm{e}}p_{\mathrm{h}}\bar{p}_{\mathrm{e}}\bar{p}_{\mathrm{h}}}\\&\times(\tilde{E},\Delta_1,\ldots,\Delta_N,).\end{aligned} \tag{40}$$

As a result, we obtain

$$\bar{\boldsymbol{\mathcal{G}}}(\tilde{E}):=\langle\boldsymbol{\mathcal{G}}(\tilde{E})\rangle=(E+\imath(1+\alpha)\gamma-\boldsymbol{\mathcal{M}})^{-1}. \tag{41}$$

Thus, with respect to the pure system, diagonal disorder just leads to the replacement of $E=\hbar\omega$ by the complex quantity $E\rightarrow E+\imath(1+\alpha)\gamma$, which leads to the expected Lorentzian broadening of the optical absorption spectrum.

V. APPLICATIONS

The Green function of the noninteracting pure wire is well known from textbooks, e.g., Economou.[29] In a sligthly rewritten form which is suitable for the analytic continuation to complex $T_0=\overline{\epsilon_0^{\mathrm{e}}}+\overline{\epsilon_0^{\mathrm{h}}}$, $T_1=\overline{t_1^{\mathrm{e}}}+\overline{t_1^{\mathrm{h}}}$, $(\Re T_1<0)$, it reads

$$G^{(0)}_{lm}(\tilde{E})=\frac{\rho_1^{|l-m|}(\tilde{E})}{\sqrt{(\tilde{E}-T_0)^2-4T_1^2}}, \tag{42}$$

where

$$\rho_1(\tilde{E})=(\tilde{E}-T_0-\sqrt{(\tilde{E}-T_0)^2-4T_1^2})/(2T_1). \tag{43}$$

$\sqrt{x}$ denotes the square root whose imaginary part has the same sign as $\Im x$, see Eqs. (33),(41).

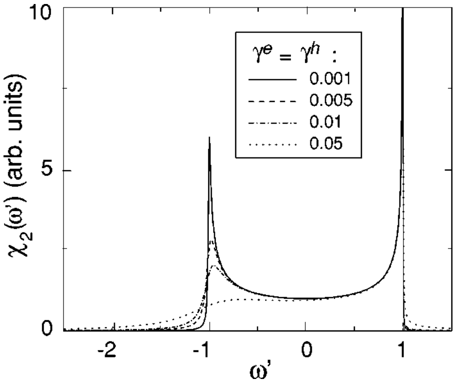

FIG. 2. Optical absorption of the noninteracting electron–hole system with varying barrier disorder. $\alpha^{\mathrm{e}}=\alpha^{\mathrm{h}}=1.1$. Energies are given in units of one half of the transition band width, lower band edge is at $\omega'=-1$.

First, we consider a local electron—hole interaction, $V_r = V_0\delta_{r,0}$, $V_0<0$. In this case Eq. (17) can be solved analytically

$$G_{00}(\tilde{E}) = \frac{G^0_{00}(\tilde{E})}{1-V_0 G^0_{00}(\tilde{E})}. \tag{44}$$

Without disorder (i.e., real T_0, T_1) the optical absorption $\chi_2 = \Im\chi$ of a wire becomes

$$\chi_2(\hbar\omega) = \frac{|W|^2}{2\pi|T_1|}\frac{\sqrt{1-\omega'^2}}{v_0^2+1-\omega'^2}, \quad |\omega'|<1, \tag{45}$$

$$\chi_2(\hbar\omega) = \frac{|W|^2}{2|T_1|}\frac{v_0}{\sqrt{1+v_0^2}}\delta(\omega'+\sqrt{1+v_0^2}), \quad \omega'<-1, \tag{46}$$

where $\omega' = (\hbar\omega - T_0)/(2|T_1|)$, $v_0 = |V_0/(2T_1)|$. W contains the interband dipole matrix element and an overlap integral between Wannier functions. A similar result has been obtained by Ishida *et al.*[7] Note that $\hbar\omega$ is measured with respect to the gap energy E_{g} of the homogeneous wire, Fig. 1.

For a quantum wire we have to replace the three-dimensional Coulomb potential by the envelope averaged potential which can be approximated quite well by[1]

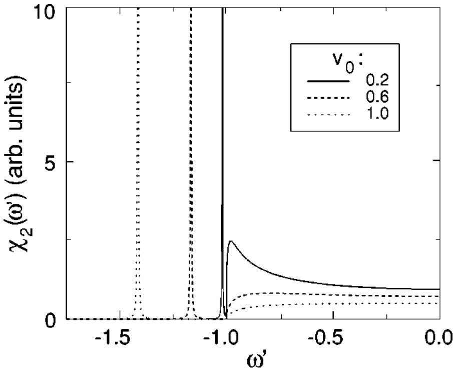

FIG. 3. Optical absorption of the pure wire with variation of the local electron–hole interaction. Energy scales as in Fig. 2.

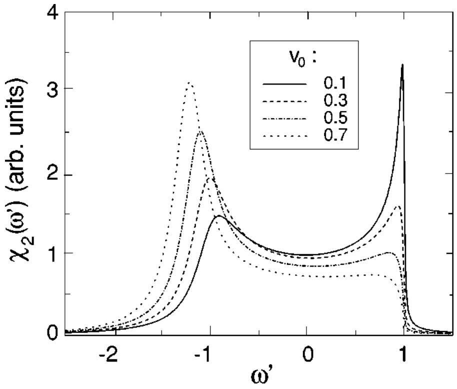

FIG. 4. Optical absorption with varying electron–hole interaction. Fixed barrier disorder, $\alpha^{\mathrm{e}}=\alpha^{\mathrm{h}}=1.1$, $\gamma^{\mathrm{e}}=\gamma^{\mathrm{h}}=0.025$. Energy scales as in Fig. 2.

$$V(z) = -\frac{e^2}{4\pi\epsilon_0\bar{\epsilon}}\frac{1}{|z|+\beta R}, \tag{47}$$

where R is the wire radius, $\beta\approx 0.3$, and $\bar{\epsilon}$ is an average dielectric constant. For a GaAs-based wire of radius $R = 50$ Å, $V(0)\approx -0.1$ eV which is approximately the full electron–hole transition bandwidth $4|T_1|$, hence $v_0\approx 0.5$.

To solve the Dyson equation Eq. (17) the effective exciton potential Eq. (47) is truncated to a finite range, $V_r = V(rb) = 0$, $|r|>s$. Then, the optical absorption, Eq. (12), is obtained numerically by solving a $(2s+1)$-dimensional linear set of equations for $G_{l0}(\tilde{E})$, $l=-s,\ldots,s$. Figures 2–6 display various examples for the perfect and disordered wire.

VI. CONCLUSIONS

The optical absorption in a quasi-one-dimensional system sensitivly depends on both the electron–hole interaction and the disorder scattering. Diagonal disorder just results in a Lorentzian smearing of the optical lines, whereas correlated diagonal/off-diagonal disorder is different: The broadening is stronger at the lower than at the upper band edge, Fig. 2. However, the shape of the absorption spectrum is drastically changed even by a tiny electron–hole interaction: The diver-

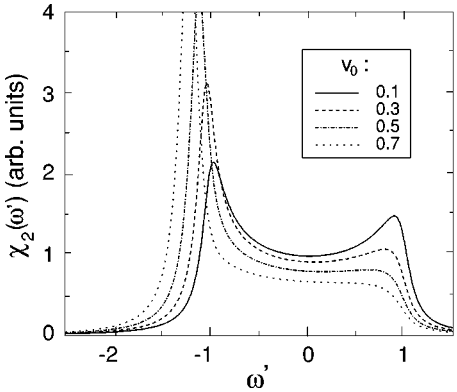

FIG. 5. Optical absorption with varying electron–hole interaction. Fixed well disorder, $(1+\alpha)\gamma=0.1$. Energy scales as in Fig. 2.

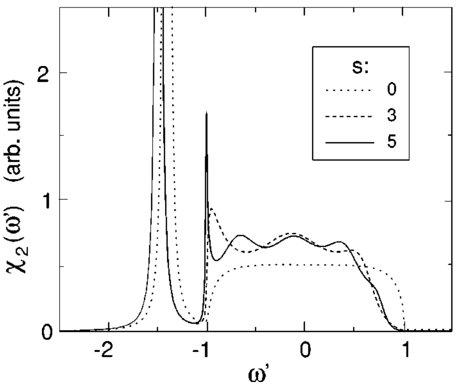

FIG. 6. Optical absorption with varying range *s* of the truncated electron–hole Coulomb interaction, $v_0 = 1$. Fixed well disorder. $\alpha^{\rm e} = \alpha^{\rm h} = 1.25$, $\gamma^{\rm e} = \gamma^{\rm h} = 0.005$. Energy scales as in Fig. 2.

gences at the band edges are completely removed so that the identification of the gap is a nontrivial problem in quasi-one-dimensional semiconductors, Figs. 3–5. For a local electron–hole interaction there is only but a single exciton bound state, Fig. 3, whereas the (truncated) Coulomb potential leads to an additional pronounced spike near the gap and an oscillatory structure within the absorption band, Fig. 6. These structures are insensitive with respect to the type of disorder.

Our approach is based on the locator expansion of the Green function (von Neumann series) whose convergence is rarely established in general. A more rigorous treatment, however, shows that Eq. (33) is indeed correct if $\alpha > 1$.[30] For $0 < \alpha < 1$, Eq. (33) leads to a negative absorption in some part of the spectrum which is definitively incorrect. It seems that the Lloyd model cannot be formulated for purely nondiagonal disorder, i.e., $\alpha = 0$. A similar problem is known for the extension of the CPA to nondiagonal disorder,[31] but it may be also due to the pathological Lorentzian probability distribution, Eq. (31), of the Lloyd model.

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