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Effect of spin variables and exciton motion on ground-state properties of the "trion"

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We solve a quantum three-body problem involving two holes and a single electron ("trion") in a two-band Hubbard model. The particles' spin and the exciton hopping matrix element are all included. We compare the results with those of a previous paper, in which these additional complications were absent, and find broad agreement. There is one novelty: The trion with singlet holes is always mobile, even in one dimension.

I. INTRODUCTION

In a recent Letter[1] (denoted I henceforth) we solved exactly a prototype quantum three-body problem consisting of two holes and an electron in a two-band Hubbard model which neglects the particle spin as well as the motion of the exciton. We found that the existence of a trion, i.e., a three-body bound state, and the magnitude of its effective mass m^*_{trion} depends sensitively on the lattice dimensionality and on the valence- to conduction-band—width ratio. References to previous literature related to this work are listed in I and will not be repeated.

The present paper has two purposes: (1) to supply the missing mathematical details leading to results in I and (2) to study the effects of the spin of the electron and holes and of an additional, "dipolar" exciton hopping term (first proposed by Heller and Marcus[2]) on the formulas for the spinless trion in I. The recoil of the exciton[3] is a particularly nontrivial modification. The *scattering states* will *not* be discussed in this paper, although they are easy to obtain (in principle).

Our conclusion is that, while spin and exciton motion may change the dynamics of the trion, many of the features described in I remain qualitatively unaltered. We will now examine the following Hamiltonian:

$$H = H_C + H_V + H_Q + H_{\text{Coul}} + H_B \ , \tag{1a}$$

where

$$H_C = -C \sum_{i,\delta,\sigma} c^*_{i,\sigma} c_{i+\delta,\sigma} \ , \quad C>0 \tag{1b}$$

$$H_V = V \sum_{i,\delta,\sigma} v^*_{i,\sigma} v_{i+\delta,\sigma} \ , \quad V>0 \tag{1c}$$

$$H_Q = -Q \sum_{i,\delta,\sigma,\sigma'} c^*_{i,\sigma} v_{i,\sigma'} v^*_{i+\delta,\sigma'} c_{i+\delta,\sigma} \ , \quad Q \geq 0 \tag{1d}$$

$$H_B = \frac{B}{2} \sum_{i,\sigma} (c^*_{i\sigma} c_{i\sigma} - v^*_{i\sigma} v_{i\sigma}) \ , \quad B>0 \tag{1e}$$

$$H_{\text{Coul}} = U_{CC} \sum_i c^*_{i\uparrow} c_{i\uparrow} c^*_{i\downarrow} c_{i\downarrow} + U_{VV} \sum_i v^*_{i\uparrow} v_{i\uparrow} v^*_{i\downarrow} v_{i\downarrow} + U_{CV} \sum_{i,\sigma,\sigma'} c^*_{i,\sigma} c_{i,\sigma} v^*_{i\sigma'} v_{i\sigma'} \ ,$$
$$U_{VV} \geq U_{CV} > 0 \ , \quad U_{CC} > 0 \tag{1f}$$

in which $i, i+\delta$ are nearest-neighbor sites, C and B the conduction- and valence-band—width parameters, and U_{CV} and U_{CC}, U_{VV} the interband and intraband electron repulsion parameters (restricted to $U_{VV} > U_{CV}$, which is normally the case in nature). The exciton hopping parameter Q is also assumed to be positive as in Ref. 3, and B is related to the band gap $E_g = B - z(C+V)$, with z the coordination number of the lattice ($z=2d$ for a d-dimensional simple cubic lattice).

If B is large enough compared to C, V, and Q, the valence band is fully occupied with two electrons of opposite spin at each site (anticommuting creation destruction operators $v^*_{i,\sigma}$, $v_{i,\sigma}$, and $\sigma = \pm\frac{1}{2}$) and the conduction band $(c^*_{i,\sigma}, c_{i,\sigma})$ is empty in the ground state which we denote by $|\Omega\rangle$.

Starting from the ground state $|\Omega\rangle$ we introduce two holes into the valence band and one electron in the conduction band. This three-particle state is then described by

$$|\Psi\rangle = \sum_{\vec{n},\vec{m}_1,\vec{m}_2} \psi(\vec{n};\vec{m}_1,\vec{m}_2) c^*_{n,\sigma} v_{m_1,\sigma_1} v_{m_2,\sigma_2} |\Omega\rangle \ , \tag{2}$$

where

$$\psi(\vec{n};\vec{m}_1,\vec{m}_2) = \begin{cases} +\psi(\vec{n};\vec{m}_2,\vec{m}_1) \ , & S=0 \\ -\psi(\vec{n};\vec{m}_2,\vec{m}_1) \ , & S=1 \end{cases}$$

and S is the total spin of the two holes—a conserved quantity in this model, and thus an important quantum number (eigenvalue $\mu \equiv 1-2S = \pm 1$). We now proceed to an exact solution of the eigenvalue problem for the bound states, provided certain simplying conditions are met.

II. EIGENVALUE EQUATION

The eigenvalue equation,

$$H\,|\,\Psi\rangle = E\,|\,\Psi\rangle$$

becomes exactly solvable if we restrict ourselves to (i) simple cubic (sc)-(bipartite) lattices which have the property that they can be divided into two sublattices Λ_1 and Λ_2 and (ii) $U_{CV}=\infty$, i.e., the Frenkel limit.

Figure 1, which compares the energy of different possible configurations of the holes and the electron, shows that because of the Frenkel limit $U_{CV}=\infty$ the excitation energy $E-E_0$ (E_0 is the ground-state energy) is finite only if also $U_{VV}=\infty$, and $U_{VV}-U_{CV}\equiv U'$ is finite. This then forces one to take $B=\infty$ with $(3B/2-U_{VV})$ finite and much larger than U' in order to maintain $|\,\Omega\rangle$ as the ground state. In these limits we have a well-defined three-particle model in which, as in the model of I, *the electron is obliged to sit on the same site as either one of the holes.* In other terms, the wave function $\psi(\vec{n};\vec{m}_1,\vec{m}_2)$ in Eq. (2) has the property

$$\psi(\vec{n};\vec{m}_1,\vec{m}_2)\neq 0$$

if and only if $\vec{n}=\vec{m}_1$ or $\vec{n}=\vec{m}_2$. For convenience we define two functions ϕ,χ,

$$\phi(\vec{n},\vec{m})\equiv\psi(\vec{n};\vec{n},\vec{m})$$

with $\vec{n}$ on sublattice Λ_1 and

$$\chi(\vec{n},\vec{m})\equiv\psi(\vec{n};\vec{m},\vec{n})$$

with $\vec{n}$ on sublattice Λ_2. Then $\psi(\vec{n};\vec{n},\vec{m})$ for $\vec{n}$ on

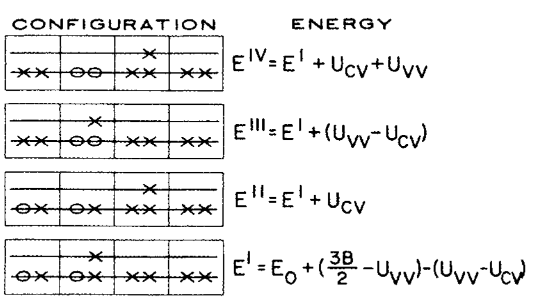

FIG. 1. Various configurations of two holes in the valence band and one electron in the conduction band (× ×, o o—2 electrons or two holes in the same site, etc.) and their energy. Ground-state energy is E_0, $3B/2$ is the energy to create the three quasiparticales, the U's are the various interactions (see text). This figure should be read from bottom up.

Λ_2 is given by

$$\psi(\vec{n};\vec{n},\vec{m})=\begin{cases}+\chi(\vec{n},\vec{m})\,, & S=0\\ -\chi(\vec{n},\vec{m})\,, & S=1\end{cases} \tag{3a}$$

and $\psi(\vec{n};\vec{m},\vec{n})$ for $\vec{n}$ on Λ_1 is given by

$$\psi(\vec{n};\vec{m},\vec{n})=\begin{cases}+\phi(\vec{n},\vec{m})\,, & S=0\\ -\phi(\vec{n},\vec{m})\,, & S=1\,.\end{cases} \tag{3b}$$

The eigenvalue equation $H\,|\,\Psi\rangle=E\,|\,\Psi\rangle$ leads then to a set of equations in the ϕ and χ.

For $\vec{m}\neq\vec{n}$, $\vec{n}+\vec{\delta}$,

$$-V\sum_{\delta'}\phi(\vec{n},\vec{m}+\vec{\delta}')-\mu Q\sum_{\delta'}\chi(\vec{n}+\vec{\delta}',\vec{m}) =\epsilon\phi(\vec{n},\vec{m})\,. \tag{4a}$$

For $\vec{m}=\vec{n}+\vec{\delta}$,

$$-V\sum_{\delta'}\phi(\vec{n},\vec{n}+\vec{\delta}+\vec{\delta}')-\mu Q\sum_{\delta'}\chi(\vec{n}+\vec{\delta}',\vec{n}+\vec{\delta}) -C\chi(\vec{n}+\vec{\delta},\vec{n})=\epsilon\phi(\vec{n},\vec{n}+\vec{\delta})\,. \tag{4b}$$

And for $\vec{m}=\vec{n}$,

$$-2V\sum_{\delta'}\phi(\vec{n},\vec{n}+\vec{\delta}')-2Q\sum_{\delta'}\chi(\vec{n}+\vec{\delta}',\vec{n}) +U'\phi(\vec{n},\vec{n})=\epsilon\phi(\vec{n},\vec{n})\ \text{ for } S=0 \tag{4c}$$

$$\phi(\vec{n},\vec{n})\equiv 0\quad\text{for } S=1 \tag{4c'}$$

where (3a) and (3b) were used, and $\mu=\pm 1$ as follows:

$$\mu=\begin{cases}1\,, & S=0\\ -1\,, & S=1\,.\end{cases}$$

The energy eigenvalue is

$$\epsilon=E-E_0-(3B/2-U_{VV})+U'\,.$$

The set of equations for $\chi(\vec{n},\vec{m})$ is obtained from Eqs. (4a)—(4c') by interchanging ϕ and χ.

This symmetry in ϕ and χ leads to two types of solutions:

(i) $\phi\equiv\chi$ (bonding)

(ii) $\phi\equiv-\chi$ (antibonding),

where the antibonding solution is mapped onto the bonding one by the substitutions $C\to -C$, $V\to V$, $Q\to -Q$, $U'\to U'$; therefore one has to solve only the bonding case.

Separating the center-of-mass motion,

$$\phi(\vec{n},\vec{m})=e^{i\vec{k}\cdot(\vec{n}+\vec{m})/2}F(\vec{r})\,,$$

where $\vec{r}=\vec{m}-\vec{n}$, and defining

$$H_0F(\vec{r}) \equiv -\sum_{\vec{\delta}'} \alpha_{\vec{k}}(\vec{\delta}')F(\vec{r}+\vec{\delta}') , \quad (5a)$$

$$H_1F(\vec{r}) \equiv -C\sum_{\vec{\delta}'} F(-\vec{\delta}')\delta_{\vec{r},\vec{\delta}'} + \left[U'F(0) - \sum_{\vec{\delta}'} \alpha_{\vec{k}}(\vec{\delta}')F(\vec{\delta}')\right]\delta_{\vec{r},\vec{0}} \quad (5b)$$

with

$$\alpha_{\vec{k}}(\vec{\delta}) = Ve^{i\vec{k}\cdot\vec{\delta}/2} + \mu Qe^{-i\vec{k}\cdot\vec{\delta}/2}$$

and

$$U' \le \infty , \quad S=0$$

$$U' = \infty , \quad S=1 .$$

Equations (4a)–(4c′) produce

$$(H_0+H_1)F(\vec{r}) = \epsilon F(\vec{r}) , \quad (6)$$

the eigenvalue equation for $F(\vec{r})$. [Note: For $S=1$ we take $U'=\infty$ in order to fulfill the boundary condition $F(0)=0$ which follows from (4c′).] Using the Green's functions associated with (5a), Eq. (6) leads immediately to a set of $(2d+1)$ linear equations for $F(0)$ and $F(\vec{\delta})$,

$$\begin{aligned} F(\vec{0}) &= -G(\vec{0},\vec{0})U'F(\vec{0}) + \sum_{\vec{\delta}'}[\alpha_{\vec{k}}(\vec{\delta}')G(\vec{0},\vec{0}) + CG(\vec{0},-\vec{\delta}')]F(\vec{\delta}') , \\ F(\vec{\delta}) &= -G(\vec{\delta},\vec{0})U'F(\vec{0}) + \sum_{\vec{\delta}'}[\alpha_{\vec{k}}(\vec{\delta}')G(\vec{\delta},\vec{0}) + CG(\vec{\delta},-\vec{\delta}')]F(\vec{\delta}') , \end{aligned} \quad (7)$$

where

$$G(\vec{r},\vec{r}') = \frac{1}{(2\pi)^d}\int d^dq \frac{e^{i\vec{q}\cdot(\vec{r}-\vec{r}')}}{\epsilon_{\vec{k}}(\vec{q})-\epsilon} , \quad (8)$$

$$\epsilon_{\vec{k}}(\vec{q}) = -\sum_{\delta}\left[(V+\mu Q)\cos\left[\frac{\vec{k}\cdot\vec{\delta}}{2}\right]\cos(\vec{q}\cdot\vec{\delta}) + (V-\mu Q)\sin\left[\frac{\vec{k}\cdot\vec{\delta}}{2}\right]\sin(\vec{q}\cdot\vec{\delta})\right] . \quad (9)$$

Part of the $\vec{k}$ dependence in Eq. (8) factorizes,

$$G(\vec{r},\vec{r}') = e^{[i\vec{\phi}(\vec{k})/2]\cdot(\vec{r}-\vec{r}')}\frac{1}{(2\pi)^d}\int d^dq \frac{e^{i\vec{q}\cdot(\vec{r}-\vec{r}')}}{-\sum_{\delta}|\alpha_{\vec{k}}(\vec{\delta})|\cos(\vec{q}\cdot\vec{\delta})-\epsilon} , \quad (10)$$

where each component satisfies

$$\tan\left[\frac{\phi_j(\vec{k})}{2}\right] = \frac{V-\mu Q}{V+\mu Q}\tan\left[\frac{k_j}{2}\right] . \quad (11)$$

For $\vec{k}=(K,K,\ldots,K)$ the set of equations (7) can be reduced, using the symmetry leading to $F(\pm\vec{\delta}) \equiv F_\pm$ for all primitive translation vectors $\vec{\delta}=(0,\ldots,+1,\ldots,0)$ for the lowest bound state. Using this in Eq. (7) we get nontrivial solution if the following 3×3 secular determinant vanishes:

$$\det|M_{ij}| = 0 , \quad (12)$$

where

$$M_{11} = -(1+U'G_0) ,$$

$$M_{12} = e^{i\phi(K)/2}d(|\alpha_K|G_0+CG_1) ,$$

$$M_{13} = e^{-i\phi(K)/2}d(|\alpha_K|G_0+CG_1) ,$$

$$M_{21} = -U'e^{i\phi(K)/2}G_1 ,$$

$$M_{22} = e^{i\phi(K)}[d|\alpha_K|G_1+(d-1)CG_{11} + CG_2 - e^{-i\phi(K)}] ,$$

$$M_{23} = [d|\alpha_K|G_1+(d-1)CG_{11}+CG_0] ,$$

$$M_{31} = -U'e^{-i\phi(K)/2}G_1 ,$$

$$M_{32} = [d|\alpha_K|G_1+(d-1)CG_{11}+CG_0] ,$$

$$M_{33} = e^{-i\phi(K)}[d|\alpha_K|G_1+(d-1)CG_{11} + CG_2 - e^{i\phi(K)}] ,$$

where

$$G_m(\epsilon,K) = \frac{1}{(2\pi)^d}\int d^dq \frac{\frac{1}{d}\sum_{j=1}^{d}\cos(mq_j)}{-2|\alpha_K|\sum_{j=1}^{d}\cos(q_j)-\epsilon} , \quad (13)$$

$$G_{11}(\epsilon,K) = \frac{1}{(2\pi)^d}\int d^dq \frac{\frac{1}{d(d-1)}\sum_{j\neq k}^{d}\cos q_j \cos q_k}{-2|\alpha_K|\sum_{j=1}^{d}\cos(q_j)-\epsilon} , \quad (14)$$

and

$$|\alpha_K| = (V^2+Q^2+\mu 2VQ\cos K)^{1/2} . \quad (15)$$

III. RESULTS AND DISCUSSION

The cases $S=0$ and 1 have to be treated separately.

(1) $S=1(\mu=-1)$.

With the use of the relations

$$G_1 = -\frac{1}{2|\alpha_K|d}(1+\epsilon G_0) ,$$

$$G_0+G_2+2(d-1)G_{11} = \frac{1}{2|\alpha_K|^2 d}\epsilon(1+\epsilon G_0) ,$$

which can be easily proven, the condition (12) simplifies for $U'=\infty$ to

$$\cos\phi(K)f(\epsilon,K)+g(\epsilon,K)=0 , \quad (16a)$$

where

$$f(\epsilon,K)=\frac{1}{C}\left[G_0(\epsilon,K)[G_0(\epsilon,K)-G_2(\epsilon,K)] + \frac{1}{2|\alpha_K|^2 d}[1+\epsilon G_0(\epsilon,K)]\right] , \quad (16b)$$

$$g(\epsilon,K)=\frac{1}{2|\alpha_K|^2 d}[G_0(\epsilon,K)-G_2(\epsilon,K)] \times[1+\epsilon G_0(\epsilon,K)]+\frac{1}{C^2}G_0(\epsilon,K) , \quad (16c)$$

which has the same structure as the result for the spinless trion (see Ref. 1), to which it reduces in the limit $Q=0$.

For $K=0$ and π, Eq. (16a) factorizes,

$$\left[G_0-G_2\pm\frac{1}{C}\right]\left[G_0\pm\frac{C}{2|\alpha_K|^2 d}(1+\epsilon G_0)\right]=0 , \quad (17)$$

where the upper sign refers to $K=0$ and the lower to π.

For $\epsilon < -2|\alpha_K|d$, the lower band edge, we have

$$G_0(\epsilon,K)-G_2(\epsilon,K)>0 ,$$

$$G_0(\epsilon,K)>0 ,$$

and

$$\frac{C}{2|\alpha_K|^2 d}[1+\epsilon G_0(\epsilon,K)]<0 .$$

Thus the lowest bound-state energy is determined by

$$G_0(\epsilon,0)=-\frac{1}{\epsilon+2\alpha_0/C} \quad \text{for } K=0 \quad (18a)$$

and

$$G_0(\epsilon,\pi)-G_2(\epsilon,\pi)=\frac{1}{C} \quad \text{for } K=\pi . \quad (18b)$$

From Eq. (18) we immediately find the critical $\nu_K \equiv |\alpha_K|/C$ such that for all $\nu_K<(\nu_K)_{\rm crit}$ there is a bound state,

$$(\nu_0)_{\rm crit}=\left[\frac{V-Q}{C}\right]_{\rm crit}=1-\frac{1}{W_d} \quad (19a)$$

and

$$(\nu_\pi)_{\rm crit}=\left[\frac{V+Q}{C}\right]_{\rm crit}=\frac{1}{d}S_d , \quad (19b)$$

where W_d is Watson's integral[4] and S_d a modified[5] Watson integral (see also I); $S_1=1$ and $S_2=(\pi/2-1)(4/\pi)$. Thus we get at $K=0$ and π the same critical values as for the spinless case without exciton hopping, but with a K-dependent ν_K.

Differentiating (16a) twice with respect to K, we get the effective mass of the trion,

$$m^*_{\rm trion}=\frac{\dfrac{\partial}{\partial\epsilon}[f(\epsilon,K)+g(\epsilon,K)]}{\left[\dfrac{V+Q}{V-Q}\right]^2 f(\epsilon,K)-\dfrac{\partial^2}{\partial K^2}[f(\epsilon,K)+g(\epsilon,K)]} \quad (K=0) , \quad (20)$$

where we used $d\phi(K)/dK=(V+Q)/(V-Q)$ at $K=0$. Even though we calculate m^* along the $(111\ldots)$ direction, it is a scalar for a cubic lattice and therefore the result (2) is more general than the derivation would seem to indicate. The square bracket in the denominator, which vanishes for $Q=0$, has (at $\epsilon=-2|\alpha_0|d$ for $d=1$, 2, 3, and 4) the same singularity as the numerator. Therefore, for $Q\neq 0$ the effective trion mass is finite at $\nu_0=(\nu_0)_{\rm crit}$ in contrast to the result in I for $Q=0$ (see also Fig. 3 in I).

The one-dimensional case can be solved explicitly using

$$G_m[\epsilon(\lambda),K]=\frac{1}{2|\alpha_K|\sinh\lambda}e^{im(\phi_K/2-\lambda)} , \quad (21)$$

$$\epsilon(\lambda) = -2|\alpha_K|\cosh\lambda \, . \quad (22)$$

Equations (16a)–(16c) lead to the solution

$$e^{-\lambda} = \frac{|\alpha_K|}{C} \, ,$$

$$\epsilon(K) = -C\left[1 + \left(\frac{V}{C}\right)^2 + \left(\frac{Q}{C}\right)^2 - 2\frac{V}{C}\frac{Q}{C}\cos K\right] ,$$

leading to

$$m^*_{\text{trion}} = -\frac{C}{2VQ} \, .$$

(Note *minus* sign.) Thus there is a bound state if and only if

$$\frac{|\alpha_K|}{C} < 1 \, ,$$

which is identical to (19a) and (19b) for $K=0$ and π, respectively, with the use of $W_1 = \infty$. Also, the result for the trion mass shows that the effective mass is finite at $|\alpha_0|/C = (V+C)/C = 1$ for $Q \neq 0$.

(2) $S=0$ ($\mu=1$).

Because the determinantal condition (12) is too complicated for arbitrary U', we will only discuss Eq. (12) for $U'=0$, but all d. We get from Eq. (12) for $U'=0$,

$$\cos\phi(K)\tilde{f}(\epsilon,K) + \tilde{g}(\epsilon,K) = 0 \, , \quad (23a)$$

where

$$\tilde{f}(\epsilon,K) = \frac{1}{C}\left[\left(\frac{1}{|\alpha_k|} \frac{\epsilon}{2|\alpha_K|d} - \frac{1}{C}\right)[1+\epsilon G_0(\epsilon,K)] + G_2(\epsilon,K) - G_0(\epsilon,K)\right] , \quad (23b)$$

$$g(\epsilon,K) = [G_0(\epsilon,K) - G_2(\epsilon,K)][1+\epsilon G_0(\epsilon,K)] \times \left(\frac{1}{|\alpha_K|} \frac{\epsilon}{2|\alpha_K|d} - \frac{1}{C}\right) - \frac{1}{C^2} \, . \quad (23c)$$

As for $S=1$, one proves that for $d=1$ and 2 there exists a bound state at $K=0$ for *all* $|\alpha_0|/C = (V+Q)/C > 0$. We have not discussed the effective mass of the trion for all d, but believe that the one-dimensional behavior, which we study explicitly, is characteristic of all d.

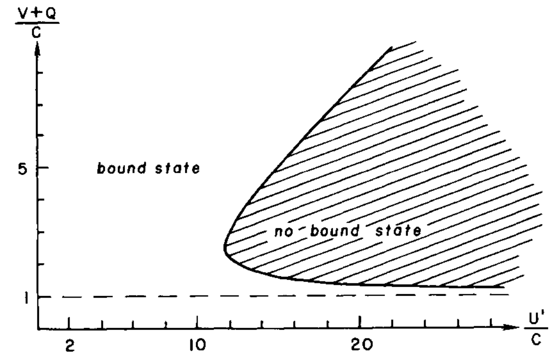

FIG. 2. Phase diagram indicating regions when trion bound state exists and where it disappears (shaded region). This is based on a calculation for $d=1$, $S=0$ ($S=1$ corresponds to $U'=\infty$ limit.)

The one-dimensional case can be discussed for *arbitrary* U'. From Eq. (12) we get

$$\left(\frac{|\alpha_K|}{C}\right)^2 e^{3\lambda} + \frac{|\alpha_K|}{C}\left(\frac{U'}{C} - 1\right)e^{2\lambda} - \left[\left(\frac{|\alpha_K|}{C}\right)^2 (1 + 2\cos\phi_K) + \frac{U'}{C}\right]e^{\lambda} - \frac{|\alpha_k|}{C} = 0 \, , \quad (24)$$

where we substituted Eqs. (21) and (22) into Eq. (12). Figure 2 shows the phase diagram in the $|\alpha_0|/C - U'/C$ parameter space where for $K=0$ a solution of Eq. (24) with $e^{\lambda(0)} > 1$, i.e., where a bound state exists. The zeros of Eq. (24) were obtained numerically.

Equation (24) differentiated twice with respect to K gives us $d^2\lambda/dK^2$ ($K=0$) which is needed for the calculation of the effective trion mass, which becomes

$$(m^*_{\text{trion}})^{-1} = 2C\left\{\left[\frac{V}{C}\frac{Q}{C}\Big/\left(\frac{V}{C}+\frac{Q}{C}\right)\right]\cosh\lambda(0) + \frac{V+Q}{C}\sinh\lambda(0) A\left(\frac{V}{C},\frac{Q}{C},\frac{U'}{C},\lambda(0)\right)\right\} , \quad (25)$$

where

$$A\left(\frac{V}{C},\frac{Q}{C},\frac{U'}{C},\lambda(0)\right) < \infty$$

is of a more complicated form (sufficiently such that we shall not give the explicit form here).

For $Q=0$, $V \neq 0$ the first term in the large curly brackets of Eq. (25) vanishes; so does the second one for $\lambda(0) \to 0$ [which happens if V/C and U'/C approaches the critical line $(V/C)_{\text{crit}} = h(U'/C)$ shown in Fig. 2.]

Thus the effective mass is infinite at the critical line if $Q=0$. However, for $Q \neq 0$ and $V \neq 0$ the first

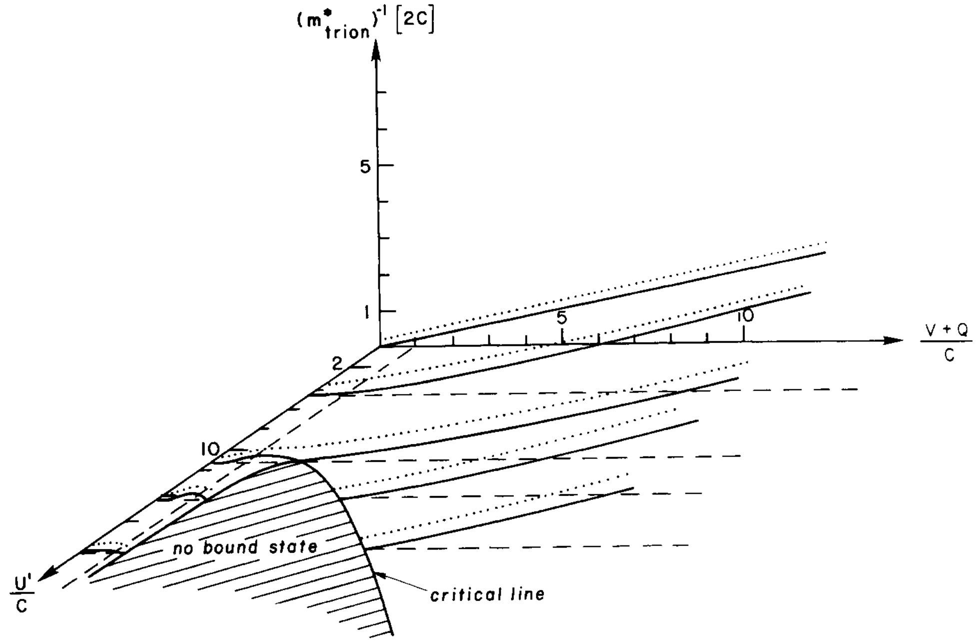

FIG. 3. Inverse trion mass as a function of $(V+Q)/C$ and U'/C for $Q=0$ (solid lines) and $Q/C=\frac{1}{2}$ (dotted lines) for the example of Fig. 2.

term in Eq. (25) is finite even for $\lambda(0)=0$, leading to a finite mass at the critical line. The numerical calculations supporting these observations are presented in Fig. 3.

In conclusion, the effect of spin depends on S, the total spin of both holes. For the holes in a triplet state ($S=1$) the problem is exactly the same as for the spinless fermions in our recent paper. However, in the singlet ($S=0$) state the trion becomes mobile in one dimension even if the exciton transfer matrix element $Q=0$. This is due to the fact that the holes in a singlet state can overlap and even cross each other.

The one-dimensional singlet case shows an interesting feature. For $U'/C \lesssim 11.65$ there exists a bound trion state at $K=0$ for *all* $(V+Q)/C$. However, for $U'/C \gtrsim 11.65$ the trion exist for small $(V+Q)/C$ and disappears at the lower $[(V+Q)/C]_{crit}$, appearing again at the upper $[(V+Q)/C]_{crit}$ (see Fig. 2). For $U'/C \rightarrow \infty$ we get exactly that the lower $[(V+Q)/C]_{crit} \rightarrow 1$ as it should, and the upper $[(V+Q)/C]_{crit} \rightarrow \infty$.

The existence of an exciton hopping term leads to a renormalization of the valence-band—width parameter, $v_K \equiv V_{renorm}(K)/C$. The critical values for v_K at $K=0$ and π for $S=1$ are identical to those for the spinless case. There is a second, probably more important effect of the Q term, namely, it makes the effective trion mass finite even in one, two, three, and four dimensions at the critical values where the bound state disappears. This is in sharp contrast to the $Q=0$ case.

We examine other many-body aspects in a separate publication.[6]

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[5] S_1 is trivial, but S_2 is not. The exact value for S_2 was calculated for us by J. Ball (private communication). We thank him for this helpful contribution. S_3 is even more difficult, but we conjecture it too can be calculated in closed form.

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