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NUMERICAL SIMULATIONS OF AN ELECTRON-EXCITON SYSTEM

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Abstract Using fermion Monte Carlo techniques we have studied the properties of a one-dimensional electron-exciton system. The zero frequency wave vector charge-density, spin-density and pairing susceptibilities were evaluated for a variety of band fillings and interaction parameters. We find that retardation and band filling are essential in determining which correlations are dominant at low temperature. While for a single chain it is possible in the strong coupling regime to have pairing correlations diverge more rapidly than charge density wave correlations, we argue that interchain couplings will lead to a 3-D charge density wave phase.

Using recently developed techniques for numerical simulations of fermion systems, we have studied a one-dimensional electron-exciton model of the type Little[1] proposed as a possible high temperature superconductor. We find that band filling and retardation play essential roles in determining whether the $2p_F$ charge density wave or single pairing susceptibility diverges most rapidly as the temperature is reduced. Here we review[2] some of the results we have obtained and conclude by commenting on the difficulty of achieving superconductivity in a 3-D array of such weakly coupled chains.

The model we have studied has the Hamiltonian

$$H = \sum_{\sigma \ell} \left[- t\left(d^{+}_{zz\sigma\ell+1} \, d_{zz\sigma\ell} + \text{h.c.} \right) - \mu n_{zz\sigma\ell} \right]$$

$$+ \sum_{\ell} \left[-\bar{t}\left(d^{+}_{xz\ell} p_{z\ell} + \text{h.c.} \right) + \epsilon_{xz} n_{xz\ell} + \epsilon_{pz} n_{pz\ell} \right]$$

$$+ \sum_{\ell} \left[U n_{zz\uparrow\ell} n_{zz\downarrow\ell} + \bar{U} n_{zz\ell} n_{xz\ell} \right] \qquad (1)$$

The first two terms describe a two-dimensional tight binding d_{zz}-band filled to a density $\rho = \langle n_{zz} \rangle$ set by the chemical potential μ. The next two terms describe the hybridization of a d_{zx} orbital on each site with its surrounding ligand represented by p_z, and the last two terms are the onsite Coulomb interactions among the d-orbitals.[3] The hybridization overlap $\bar{t}$ mixes the $d_{xz} - p_z$ orbitals forming bonding and antibonding states separated by an energy of order $2\bar{t}$ when $\epsilon_{xz} + \bar{U}\langle n_{zz} \rangle - \epsilon_{pz} \simeq 0$. Here we will assume that the bonding orbital always lays below the fermi level and the antibonding orbital well above.

The $d_{xz} - p_z$ system forms the polarizable "side chain" in Little's model. A d_{zz} electron can interact with this "side chain" via the Coulomb repulsion $\bar{U}$ producing a virtual admixture of the anti-bonding state and polarizing the $d_{xz} - p_z$ system. The polarization can then scatter a second d_{zz} electron giving rise to an attractive electron-electron interaction when the energy transfer is less than the exciton splitting $2\bar{t}$. To second order in $\bar{U}$, the effective interaction has the form

$$\frac{\bar{U}^2 \bar{t}}{\omega^2 - (2\bar{t})^2 + i\delta} \qquad (2)$$

When $\omega = 0$, this reduces to $-\bar{U}^2/4\bar{t}$. It is this type of excitonic mediated attractive interaction which Little suggested could give rise to high temperature superconductivity. However, as is now well known, a one-dimen-

sional electron gas has a variety of competing instabilities,[4-5] and a central question is whether such a system will exhibit a $2p_F$ charge-density-wave CDW instability and/or single pairing SP correlations. We note also that in the absence of $\bar{U}$, the system described by Eq. (1) with U present will exhibit spin density wave SDW correlations.

In order to determine the behavior of this system, we have studied the zero frequency wave-vector susceptibilities characterizing these different types of instabilities.[6]

$$\mathrm{CDW} = \frac{1}{N} \sum_{\ell j \sigma \sigma'} e^{iq(\ell - j)} \int_0^\beta d\tau \left[\langle n_{\ell\sigma}(\tau) n_{j\sigma'}(0) \rangle - \langle n_{\ell\sigma}(\tau) \rangle \langle n_{j\sigma'}(0) \rangle \right]$$

$$\mathrm{SP}(q) = \frac{1}{N} \sum_{\ell j} e^{iq(\ell - j)} \int_0^\beta d\tau \langle d^+_{\ell\downarrow}(\tau) d^+_{\ell\uparrow}(\tau) d_{j\uparrow}(0) d_{j\downarrow}(0) \rangle \qquad (3)$$

$$\mathrm{SDW}(q) = \frac{1}{N} \sum_{\ell j} e^{iq(\ell - j)} \int_0^\beta d\tau \langle (n_{\ell\uparrow}(\tau) - n_{\ell\downarrow}(\tau))(n_{j\uparrow}(0) - n_{j\downarrow}(0)) \rangle$$

From both exact solutions of particular models[7] and renormalization group analyses[5] one expects these susceptibilities for an infinite chain to develop power law singularities $(t/T)^{\mu_\alpha}$ as the ratio of the temperature to the band hopping parameter t goes to zero. If, for example, $\mu_{CDW} > \mu_{SP}$, one says that the low temperature phase is CDW.

Our numerical simulations were constructed by writing the partition function as

$$Z = \mathrm{Tr} \prod_{i=1}^{L} e^{-\Delta\tau H} \qquad (4)$$

and using the small parameter ($\Delta\tau$ x energy) to approximately separate the various parts of H. Then the inter-

action terms U and $\bar{U}$ were linearized by means of a discrete Hubbard-Stratonovich transformation.[8] For example

$$e^{-\Delta\tau U n_{\ell\uparrow}(\tau) n_{\ell\downarrow}(\tau)} = \sum_{\sigma_\ell(\tau)=\pm 1} e^{\lambda\sigma_\ell(\tau)(n_{\ell\uparrow}(\tau) - n_{\ell\downarrow}(\tau) - \frac{\Delta\tau U}{2}(n_{\ell\uparrow}(\tau) - n_{\ell\downarrow}(\tau))} \tag{5}$$

with $\lambda = 2\,\mathrm{arctanh}(\sqrt{\tanh(\Delta\tau U/4)})$. The fermions were then traced out reducing the problem to evaluating sums over all the $\sigma_\ell(\tau)$ U-variables and $\bar{\sigma}_\ell(\tau)$ $\bar{U}$-variables of a determinant

$$Z = \sum_{\{\sigma_\ell(\tau),\bar{\sigma}_\ell(\tau)\}} \det\left(1 + T\, e^{-\int_0^\beta h\{\sigma_\ell(\tau),\bar{\sigma}_\ell(\tau)\}}\right) \tag{6}$$

Here $h\{\sigma_\ell(\tau),\bar{\sigma}_\ell(\tau)\}$ describes the motion of a single electron in a random space-τ field determined by the $\{\sigma_\ell(\tau),\bar{\sigma}_\ell(\tau)\}$ variables. The sums in Eq. (6) are done using a Monte Carlo importance sampling technique described in Ref. 9 and the correlation functions given by Eqs. (3) evaluated.

A variety of checks using exact solutions for small systems as well as known solutions for special cases of the infinite chain provide a basis for ascertaining that the simulation is working. This has been done, but here we will simply proceed by showing results as the different parts of H, Eq. (1), are turned on and argue that they make sense physically. Figure 1 shows CDW(q) versus q at different temperatures for a twenty-site non-interacting system [10] ($U = \bar{U} = 0$) which has a one-quarter filled band ($\rho = 0.5$). Here we measure energies in terms of the hopping parameter t. As the temperature is lowered, the well-

known growth of the $2p_F$ peak is clearly evident. A plot of the peak height CDW($2p_F$) versus $\ell n(\beta)$ gives a linear curve (until the coherence length becomes comparable with the lattice size) with slope $N(0) = (\pi v_F)^{-1} = (\sqrt{2}\pi t)^{-1}$.

Next, suppose U is turned on but $\bar{U}$ is kept equal to zero. Results[10] for CDW(q) with different values of U are shown in Fig. 2a. As U increases, the $2p_F$ peak decays and a peak at $4p_F$ grows. For $U = \infty$, the charge degrees of the system behave as if the band were half filled with spinless fermions giving rise to a peak at $q = \pi = 4p_F$. The SDW(q) susceptibility for this same case is shown in Fig. 2b, and one clearly sees the growth of a spin density wave at $2p_F$ as one expects on physical grounds.

Next, U is set to zero and $\bar{U}$ is turned on. Figures 3a and b show that for the one-quarter filled case both the SP(0) and CDW($2p_F$) responses are enhanced by the exciton coupling. In order to determine which response is diverging most rapidly as the temperature is lowered, one can plot the peak heights SP(0) and CDW($2p_F$) versus $\ell n(\beta)$. In doing this throughout our work we have scaled the lattice size N and the inverse temperature β so that $\beta = N/4$. A particular case for which we know the answer is the half-filled $\rho = 1$ band where Umklap processes make CDW($2p_F$) dominate. Figure 4, SP(0) and CDW($2p_F$) are plotted versus $\ell n(\beta)$ for $\rho = 1.0$. Here the simulation clearly shows that the system is in a CDW state at low temperatures.

For a non-half-filled band, such as the $\rho = 0.5$ case shown in Figure 3, the situation is less clear. In order to explore this in more detail, we studied the effects of retardation by keeping $\bar{U}$ fixed and varying $\bar{t}$. The behavior of SP(0) and CDW($2p_F$) for the exciton model, Eq. (1), are shown as the solid curves in Figure 5. The dashed

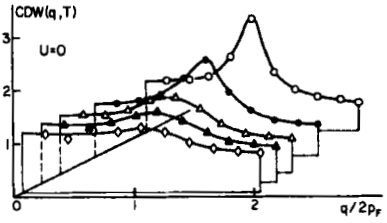

FIGURE 1 CDW(q) versus q for a free d_{zz}-band normalized to its zero temperature q = 0 value $2/\pi v_F$. The five curves correspond front to back to $\beta = 3, 3.75, 4.5, 7.25$ and 14.5, respectively (for $4t = 0.5$ eV the corresponding temperatures vary from 500 to 100 K in steps of 100 K).

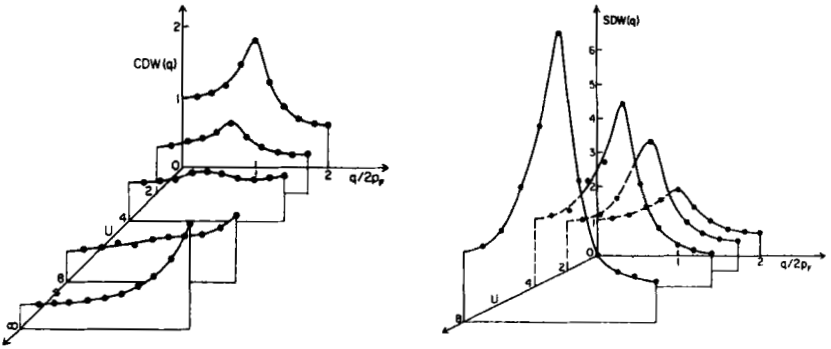

FIGURE 2 (a) Charge-density, and (b) spin-density susceptibilities for various values of U at $\beta = 7.25$.

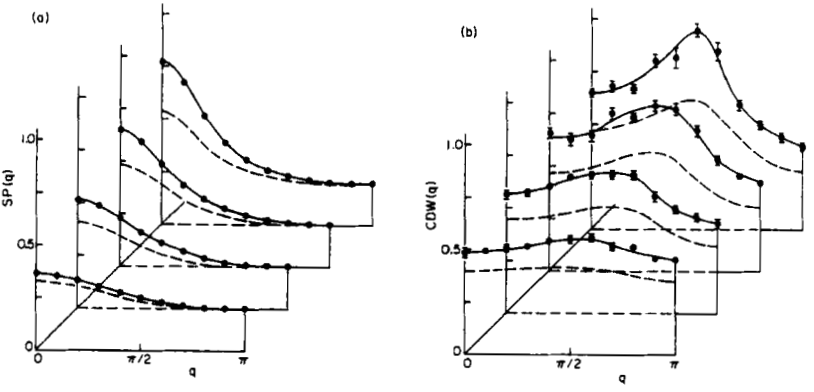

FIGURE 3 (a) SP(q) and (b) CDW(q) versus q for a 20-site lattice at $\beta = 2,3,4,5$ and $\bar{U} = \sqrt{8}$, $\bar{t} = 2$, $\epsilon = \epsilon_{pz} - \epsilon_{xz} = \bar{U}/2$. The dashed curves show the susceptibilities for the non-interacting d_{zz} band.

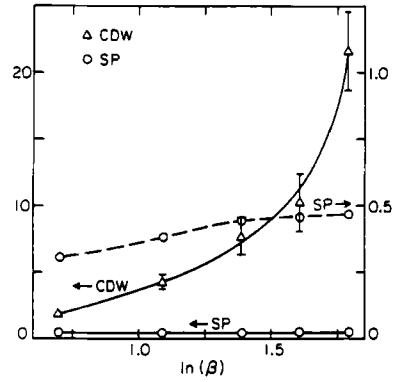

FIGURE 4 CDW($2p_F$ and SP(0) versus $\ell n(\beta)$ for $\rho = 1$, $\bar{t} = 0.5$, $\bar{U} = \sqrt{8}$ and $\epsilon = \bar{U}$. The dashed line shows SP(0) on the enlarged right-hand scale.

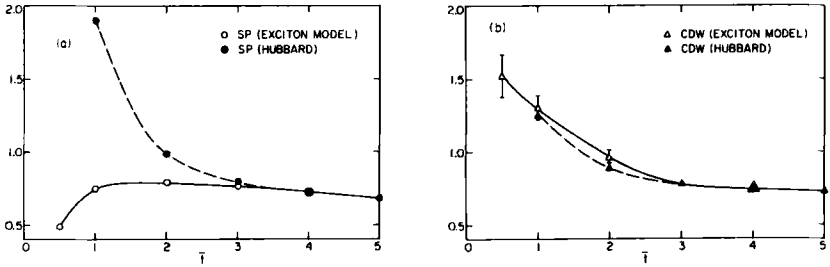

FIGURE 5 (a) SP(0) and (b) CDW($2p_F$) versus $\bar{t}$ with $\beta = 5$, $\bar{U} = \sqrt{8}$, $\epsilon = \bar{U}/2$, $U = 0$ and $\rho = 0.5$. The dashed lines show the results for an attractive Hubbard model with $U_{eff} = -\bar{U}^2/4\bar{t}$.

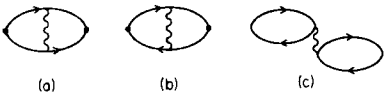

FIGURE 6 First order (a) SP correction, (b) vertex correction for CDW, and (c) bubble correction to CDW.

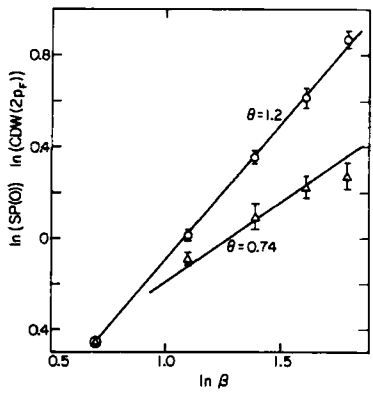

FIGURE 7 $\ell n(SP(0))$ and $\ell n(CDW(2p_F))$ versus $\ell n\beta$ for an attractive Hubbard with an effective $U_{eff} = -\bar{U}^2/4\bar{t} = -2$ and $\rho = 0.5$.

curves are the results obtained from the simulation of an attractive Hubbard model with an effective U equal to $-\bar{U}^2/4\bar{t}$. For the exciton model, retardation suppresses the SP(0) response while leaving CDW($2p_F$) largely unaffected. This can be qualitatively understood by considering the low order perturbation theory graphs shown in Figure 6. Here the wavy line represents the exciton interaction Eq. (2). In the pair-pair propagator (Fig. 6a) and the polarization vertex correction (Fig. 6b), the interaction carries a frequency which is summed over and reduces the strength of the interaction[11] when it becomes comparable to $2\bar{t}$. However, in the zero frequency contribution of Figure 6c to CDW(q), the exciton interaction enters with its full strength $-\bar{U}^2/4\bar{t}$. Thus the SP contribution of Figure 6a is suppressed by retardation while the CDW contribution of Fig. 6c is not, and, in addition, the negative contribution from Fig. 6b is suppressed, further enhancing the CDW response.[12]

Were it not for retardation effects, SP(0) would in fact diverge more rapidly than CDW($2p_F$) for this $\rho = 0.5$ case as indicated by the dashed curves in Figure 5 obtained for the attractive Hubbard model. Thus, in seeking a regime in which pairing correlations are stronger than charge density correlations, it is clear that we need a band which is not one-half full and a large $\bar{t}$ so that retardation effects are minimized. For $\bar{t}$ of order the bandwidth 4t, retardation is negligible as shown in Figure 5 where the results of the simulation for the exciton model are essentially identical to those obtained for an attractive Hubbard model with an effective interaction $-\bar{U}^2/4\bar{t}$. Figure 7 shows SP(0) and CDW($2p_F$) for an attractive Hubbard model with $\rho = 0.5$ and $\bar{U}^2/4\bar{t} = -2$. The pairing response SP(0) clearly diverges more rapidly

than CDW($2p_F$). The straight lines correspond to the low temperature power law exponents $\mu_{SP} = 1.2$ and $\mu_{CDW} = 0.74$ given by the renormalization group.[13] We believe the remarkably close agreement between the straight line and simulation for SP(0) is fortuitous, but it is clear from these simulations that in this parameter regime the pairing correlations grow more rapidly than the charge density wave correlations.

Now, it is unrealistic[3] to keep $\bar{U}$ and neglect U. Even taking into account the fact that these two Coulomb interactions may be screened differently and that a number of side groups can be packed around the spine, U and $\bar{U}$ are proportional.[14] Thus it is important to understand what

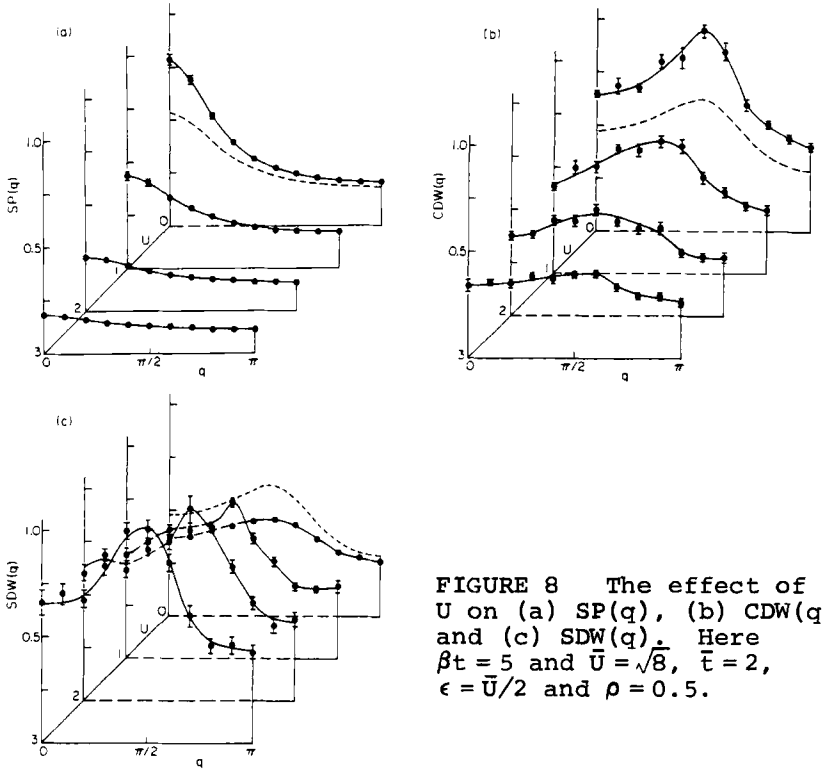

FIGURE 8 The effect of U on (a) SP(q), (b) CDW(q) and (c) SDW(q). Here $\beta t = 5$ and $\bar{U} = \sqrt{8}$, $\bar{t} = 2$, $\epsilon = \bar{U}/2$ and $\rho = 0.5$.

happens when U is turned on. Figures 8a-8c show results for the exciton model, and we see that as U increases both the SP and CDW susceptibilities are suppressed while the spin density wave SDW response at $2p_F$ emerges. Basically the effective interaction $-\bar{U}^2/4\bar{t} + U$ has become positive. In order to have pairing correlations dominate, we need to have $\bar{t}$ of order the bandwidth and $-\bar{U}^2/4\bar{t} + U < 0$. If we take $U = \bar{U}/4$, this implies that $\bar{U}$ must also be larger than the bandwidth. Thus we are in the strong-coupling limit where the onsite energies are large compared to t.

In this strong-coupling regime it is appropriate to first solve the single site problem. For a partially filled band $\rho \neq 0$ or 2, the zero and doubly occupied d_{zz} states are degenerate due to the polarizability of the $d_{xz} - p_z$ side groups and the value of the chemical potential. The $\binom{N}{N\rho/2}$ degenerate ways of placing the $N\rho/2$ pairs on N lattice sites is lifted in second order by

$$H_t \frac{1}{E_o - H_o} H_t \quad , \tag{7}$$

where $H_t = -t \sum_l \left(d^+_{zz\sigma l+1} d_{zz\sigma l} + \text{h.c.} \right)$ is the hopping term, H_o is the sum of the single site Hamiltonians, and E_o is the unperturbed ground state energy. Denoting an empty site by $S_z = -\frac{1}{2}$ and a paired site by $S_z = \frac{1}{2}$, this problem can be mapped onto an anisotropic Heisenberg model[15-16]

$$H = \frac{J_x}{2} \sum_l \left(S^+_{l+1} S^-_{l+1} S^+_l \right) + J_z \sum_l S^z_{l+1} S^z_l \tag{8}$$

with J_x and J_z functions of $\bar{t}$, $\bar{U}$ and U. Here J_x represents a pair transfer coupling, and J_z arises from the blocking of virtual single particle hopping processes which can lower the energy of a pair adjacent to an empty site.

It turns out[2] that $J_z > J_x$ so that for the half-filled band $\sum_\ell \langle S_\ell^z \rangle = 0$, the ground state is antiferromagnetically ordered implying a CDW wave as we have already seen, Figure 4. However, for $\rho \neq 1$ $\left(\frac{1}{N}\sum_\ell \langle S_\ell^z \rangle \neq 0\right)$, Haldane[17] has shown that for a certain range $J_z^c > J_z > J_x$ the transverse and longitudinal correlations decay algebraically in the ground state, and it follows that in this case $\mu_{SP} > \mu_{CDW}$ for the exciton model. In particular, for $\rho < 0.6$, J_z^c goes to ∞ and thus, for example, for a one-quarter filled band $\rho = 0.5$ the strong coupling theory predicts that $\mu_{SP} > \mu_{CDW}$, and both SP(0) and CDW($2p_F$) diverge in a manner similar to the results shown in Fig. 7.

In this strong-coupling limit each site becomes a pairing center, and the band term H_t provides a Josephson-like tunneling coupling J_x between the sites as well as an interaction term J_z. This picture of local "Schafroth-Blatt-Butler"-like[18] molecular sized pairs forming a condensate (in this 1-D case a condensate with algebraically decaying correlations) can be clearly seen in "world line" Monte Carlo configurations.[19]

Thus, for a single chain with both U and $\bar{U}$, it is possible to have the SP(0) susceptibility diverge more rapidly than CDW($2p_F$) if $\bar{t}$ and $\bar{U}$ are both comparable or larger than the bandwidth 4t and the band is less than half filled (e.g., $\rho = 0.5$). However, under these conditions <u>both</u> susceptibilities exhibit power law divergences. It is only that μ_{SP} is somewhat larger (say 25% to 50%) than μ_{CDW}. However, the interchain coupling between the charge density waves can be mediated by a direct Coulomb interaction $V_\perp$ which is of order $(V_\perp/t)$ while the interchain pair field coupling varies as $t_\perp^2/(\bar{U}t)$ where $t_\perp$ is the interchain hopping. Since $\bar{U} > t$, the pair coupling is smaller than $(t_\perp/t)^2$. Thus, while $(V_\perp/t)$ can be of

order unity, $(t_\perp/t)^2 < 10^{-2}$ for weakly coupled chains and hence, even if the pairing response of a single chain SP(0) is stronger than the charge density wave response CDW($2p_F$), the large disparity in interchain coupling should in general lead to a 3-D CDW ordering.

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