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Numerical Simulations
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Monte Carlo Studies of the Quantum XXZ Model in Two Dimensions.* E. LOH, Jr. and D.J. SCALAPINO, Univ. of California, Santa Barbara and P. GRANT, IBM Res. Lab. San Jose--Monte Carlo simulation techniques have been used to study the spin-½ XXZ model in two dimensions. By varying the $S^z - S^z$ coupling, we studied the system as it changed from an XY model through isotropic Heisenberg to Ising. Energies and specific heats were measured as functions of temperature. Spin-spin correlation functions and the helicity modulus have also been calculated. Using the data for the correlation functions and the specific heat, a finite-sized scaling analysis of the model was carried out. Results will be reported.

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Prefer
Standard Session

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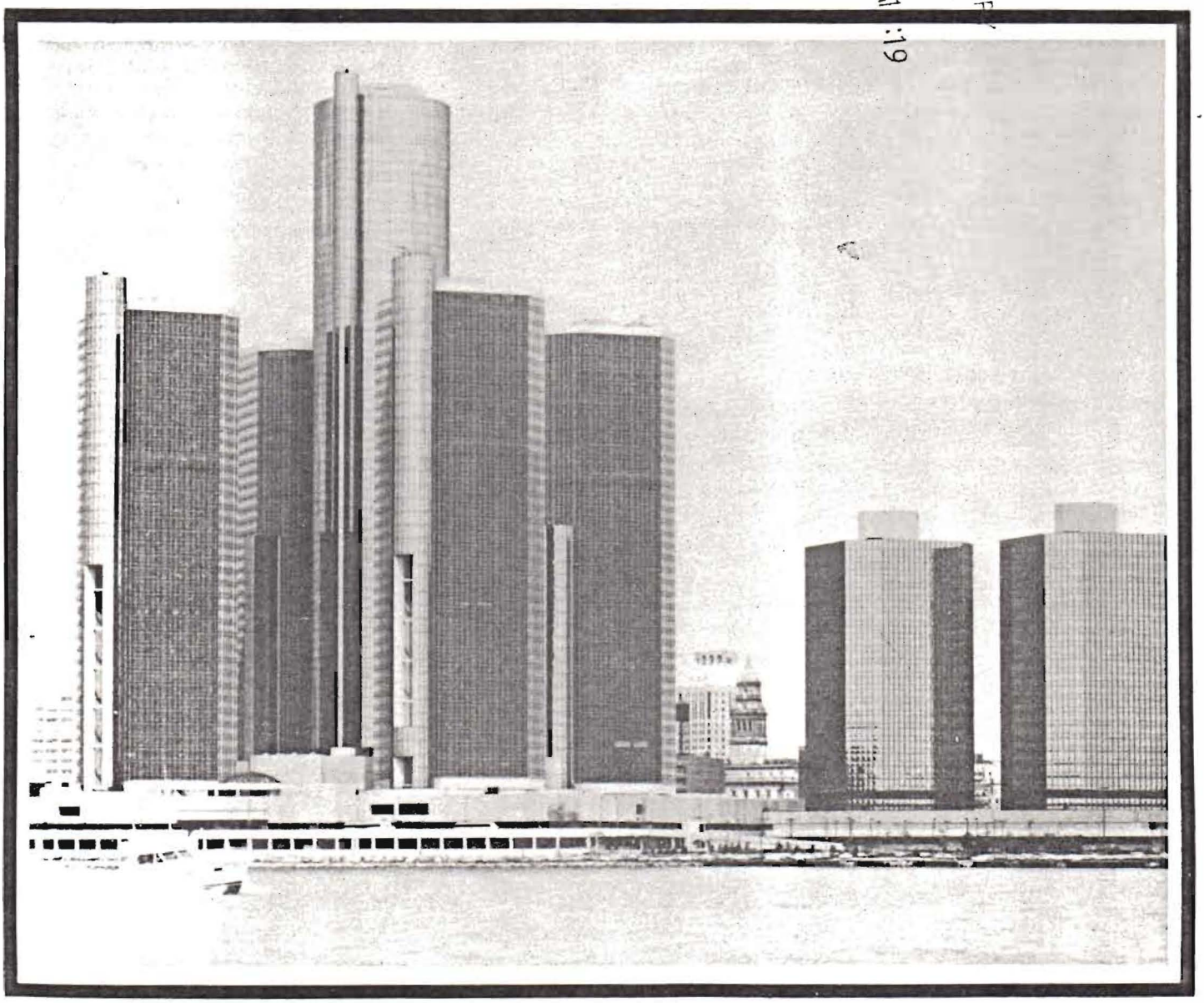

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Gaussian orbitals $a(\vec{r} - \vec{R})$ centered at the sites $\vec{R}$ of the b.c.c. lattice, with up spins on one simple cubic sublattice, down spins on the other. I show that at small interparticle separation parameter r_s, Ψ is a large-and spin-density-wave state, contrary to previous belief, and Ψ is an exact eigenstate of the HEG Hamiltonian for $r_s \to 0$. But the energy of Ψ is higher than the ground state energy in this limit by ~ 8%, (the Fermi surface being a cube instead of a sphere), much larger than the energy differences between Ψ and the ferromagnetic-fluid state when the latter is lower.[1] A new wave function $\Psi' = JD'$, where the occupied orbitals in D' are Bloch sums of the $a(\vec{r} - \vec{R})$ taken over the whole b.c.c. lattice, with spin up or down (both occupied), is shown to approach the exact ground state as $r_s \to 0$ and the Wigner solid as $r_s \to \infty$.

[1]D. Ceperley, Phys. Rev. B 18, 3126 (1978)

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AJ 5

Cooperative Magnetism in Metallic Jellium and in the Insulating Wigner Electron Crystal.* N.H. MARCH** and F. HERMAN, IBM San Jose Research Laboratory. -- As the interelectronic spacing r_s in jellium is increased from zero to infinity, one has at absolute zero successively paramagnetic and ferromagnetic metals, antiferromagnetic and finally ferromagnetic insulators. Using the Monte Carlo results of Ceperley and Alder,[1] in conjunction with the virial theorem, the electronic kinetic energy is followed as a function of r_s through the paramagnetic-ferromagnetic transition in the metallic phase, and the magnitude of the discontinuity ΔK is exposed and interpreted. The relation to the phenomenological theory of March et al[2] in which the order parameter is the discontinuity in the single-particle occupation probability at the Fermi surface is briefly considered. Some attention is then given to the antiferromagnetic-paramagnetic phase boundary in the insulating Wigner electron crystal, the long-range cooperative Néel type antiferromagnetism extending at T=0 over the density range corresponding to $100\, a_o < r_s < 70\, a_o$, where a_o is the Bohr radius. Using an approximate theory of the Néel temperature due to Carr,[3] it is established that one is dealing with cooperative antiferromagnetism in the milli-degree Kelvin range.

*Supported in part by ONR Contract Number N00014-79-C-0814.
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[1]D.M. Ceperley and B.J. Alder, Phys. Rev. Letters 45, 566 (1980).
[2]N.H. March, M. Suzuki, and M. Parrinello, Phys. Rev. B 19, 2027 (1979).
[3]W.J. Carr, Phys. Rev. 122, 1437 (1961).

10:24
AJ 6 Transition from Large to Small Polarons at Two Dimensions. M.H. COHEN, Exxon Research & Engineering Co. and L.A. TURKEVICH, Princeton U. -- We study the dimensional dependence of electron self-trapping in a deformation potential Δ within adiabatic and continuum approximations:

$$H = \int \{ \frac{\hbar^2}{2m} |\nabla\psi|^2 + \tfrac{1}{2}\Delta^2 - \Delta|\psi|^2\Delta \} d^d r$$

The scaling results complement analysis of the nonlinear Schrödinger equation. The scaling results of Emin and Holstein are reproduced for d = 1 and d = 3. The disappearance of the large polaron solution (as $d \to 2^-$) and of the small polaron solution (as $d \to 2^+$) is examined in detail. The results are generalized to anisotropic (quasi-1d, quasi-2d) continua.

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AJ 7 Continuum Model of a Mixed Peierls System. S.R. SHASTRY, TATA Institute, India, and W.P. SU,* University of Illinois at Urbana-Champaign.--A model of one dimensional systems in which the electron is coupled to two types of lattice fields is discussed. The continuum model is solved using the Fermi level scheme. Depending on the relative strength of the two couplings the model reduces to polyacetylene in one limit and to a continuous chiral symmetric model in the other limit. The soliton excitations have the reversed charge-spin relations as in polyacetylene. The soliton creation energy and the energy of the gap state are variable.
*Supported by NSF DMR81-17182

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AJ 8 Monte Carlo Studies of the Quantum XXZ Model in Two Dimensions.* E. LOH, Jr. and D.J. SCALAPINO, Univ. of California, Santa Barbara and P. GRANT, IBM Res. Lab. San Jose--Monte Carlo simulation techniques have been used to study the spin-½ XXZ model in two dimensions. By varying the $S^z - S^z$ coupling, we studied the system as it changed from an XY model through isotropic Heisenberg to Ising. Energies and specific heats were measured as functions of temperature. Spin-spin correlation functions and the helicity modulus have also been calculated. Using the data for the correlation functions and the specific heat, a finite-sized scaling analysis of the model was carried out. Results will be reported.

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11:00
AJ 9 A Functional Integral Approach to a Coupled Electron-Libron System. JOAO FLORENCIO* and BERNARD GOODMAN, U.Cincinnati.--We investigate a two level electron system coupled quadratically to librons. The partition function is formulated as a functional integral over commuting and anticommuting (Grassmann) elements. After a canonical transformation is done in the original Hamiltonian, the integral over the libronic coordinates is performed in closed form. The electronic integral is then calculated in a semi-classical approximation where the classical equations are solved exactly. The free energy of the system is found to be a smooth function of the coupling constant and of the temperature. Specific heat results will also be shown. This model is of interest for systems of linear conductors based on TCNQ molecules.

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11:12
AJ 10 Monte Carlo Study of the 2-D Spinless Hubbard Model.* D.J. SCALAPINO and R.L. SUGAR, Univ. of California, Santa Barbara and W.D. TOUSSAINT, Univ. of California, San Diego--Using recently developed fermion Monte Carlo methods[1] we have carried out simulations of a gas of spinless electrons hopping on a two-dimensional lattice with a near neighbor interaction V. For a half-filled band and a repulsive interaction $V > 0$, this system undergoes a normal metal to insulating charge density wave transition as the temperature is lowered. For an attractive interaction $V < 0$, we find both a transition to a p-wave pairing state and a gas-liquid condensation depending upon the size of $|V|/t$. Results for the charge density wave and pairing susceptibilities will be used along with a finite size scaling analysis to discuss the phase diagram of this system.

[1]R. Blankenbecler, D.J. Scalapino and R.L. Sugar Phys. Rev. D 24, 2278 (1981); D.J. Scalapino and R.L. Sugar, Phys. Rev. B 24, 4295 (1981).
*This work was supported in part by DOE Contracts DE-AT03-83ER45008 and DE-AT03-81ER40029, NSF Grant PHY80-18938, and NSF Grant PHY77-27084.