Electron-hole system revisited: A variational quantum Monte Carlo study

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Properties of a model electron-hole system are studied with a variational Monte Carlo method. Energies of both the two-component plasma phase and the excitonic insulating phase are calculated. The excitonic insulating phase is stable for all densities studied, exhibiting a strong pairing state even near $r_s=2.0$, the density where the two-component plasma phase has its minimum energy. Analysis of the pair correlation functions reveals that the stabilization of the excitonic insulator traces to enhanced short range electron-hole correlations which are partially offset by reduced electron-electron correlations. In the two-component plasma phase, significant electron-hole correlation effects remain up to high density, e.g., $r_s=0.5$. [S0163-1829(96)05543-9]

In this paper, we revisit the problem of the electron-hole liquid[1] in three dimensions with a nonperturbative, variational Monte Carlo (VMC) approach. As a model system, the electron-hole liquid exhibits (at least) two phases in principle: a metallic, two-component plasma (2CP) phase at high density and an insulating, excitonic (EI) phase at low density.[2] A naive application of the Mott criterion for the metal-insulator (MI) transition, equating the Thomas-Fermi screening length to the exciton Bohr radius, gives a transition at an average spacing between electron-hole pairs of $r_s=4(12/\pi)^{2/3}=9.8$.[3,4] We find, as already suggested earlier,[5] that the excitonic insulating phase is stable to much higher densities, including around $r_s\approx 2$ near the minimum energy for the 2CP phase. We find large many-body correlation effects in an electron-hole plasma even in the high density range $r_s\sim 0.5$, which corresponds roughly to the densities at which a typical semiconductor laser operates. The role of correlation effects continues to be an important issue in theoretical models for the material gain in semiconductor lasers.[6,7] Finally, pair correlation functions obtained from VMC wave functions are significantly different from those reported earlier based on self-consistent local-field theories.[8]

In the past, the electron-hole liquids have been studied in indirect gap materials to ensure a long lifetime for ease of measurement.[1] Band degeneracies play an important role in these systems, stabilize liquid droplet phases of fixed density, and suppress excitonic pairing.[1] Short period GaAs/AlAs superlattices afford an interesting test case where the character of the conduction-band minimum depends on the period. For short periods, the conduction-band minimum is at the X point and multivalley effects enter, while for longer periods the conduction-band minimum is at the zone center giving directly allowed optical transitions. Interestingly, time resolved luminescence studies on these materials show evidence for electron-hole droplet formation only for the short period superlattices.[9] In our calculations, we find no tendency to phase separation for a direct gap material; the energy for the excitonic insulator phase is a monotonic function of r_s in the range $2<r_s<10$, suggesting that the density can be tuned smoothly throughout this range. At present, electro-optical experiments are routinely carried out on a time scale of 10 fs, much faster than the radiative recombination time in a typical direct gap semiconductor which is on the order of nanoseconds. Thus it is now possible to directly probe the photoexcited electron-hole system in a direct gap semiconductor quantum structure, before recombination happens and after thermal equilibrium is reached on a ps time scale. A recent proposal for tuning the density of an electron-hole system in two dimensions has been given.[10]

We limit ourselves to an equal-mass, two-band model system.[12] The only relevant dimensionless parameter is then r_s. Further, we ignore the small interband exchange between an electron and a hole. The Hamiltonian reads

$$H_{eh}=\sum_i \frac{\vec{P}_{i,e}^2}{2m_e}+\sum_i \frac{\vec{P}_{i,h}^2}{2m_h}+\sum_{i<j}\frac{e^2}{|\mathbf{r}_{i,e}-\mathbf{r}_{j,e}|}+\sum_{i<j}\frac{e^2}{|\mathbf{r}_{i,h}-\mathbf{r}_{j,h}|}-\sum_{i,j}\frac{e^2}{|\mathbf{r}_{i,e}-\mathbf{r}_{j,h}|}. \quad (1)$$

From now on, we take $m_e=m_h=m$, and the exciton reduced mass is $\mu=m/2$. All of our results will be reported with energy in units of the exciton Rydberg and length (r_s parameter) in units of the exciton Bohr radius.

The metallic 2CP phase of this model system has been studied extensively in the past, using the random-phase-approximation (RPA),[8,3] the Hubbard extension of RPA (HA),[8,3] and the self-consistent local-field (SCLF) theory.[8] Two versions of the SCLF theory have been used:[8] one uses HA for the electron-electron and the hole-hole local-field factors, and iterates to self-consistency the electron-hole local-field factor (partial-self-consistency, or PSC); the other reaches full self-consistency for all three local-field factors (full-self-consistency, or FSC). More recently, the Fermionic hypernetted-chain (HNC) theory[13] has also been applied to this system.[14]

However, none of these approaches can be used to study the EI phase due to the intrinsically inadequate treatment of

the multiple electron-hole scattering at short distances. Indeed, when applied to the 2CP phase at relatively low densities where such scattering is crucial, these theories are often unstable operationally, and no self-consistent solutions can be obtained.[8,14] Arguments have been put forward by Nozieres and Comte, suggesting that the EI phase is more stable than the Mott criterion indicates.[5] A mean-field theory, similar to the BCS approach to superconductivity,[15] was solved approximately via a variational ansatz for the pairing wave function.[16,5,17,18] However, further correlation effects are difficult to include.

In this work, we study both phases using a nonperturbative, variational method. In addition to the metallic phase, we are able to treat explicitly both the pairing and the correlation effects in the EI state. We conclude that the excitonic phase is more stable than the two-component plasma phase in the entire density range where our calculations for both can be reliably carried out. We also remark that the wave function we use for the EI insulator state evolves continuously to become a Bose condensate of excitons at low density, such as has been reported in some recent experiments on excited semiconductors.[11] However, the energy cost of breaking the phase coherence implied by such a wave function is likely very small, and we shall not focus here on the possible superfluid nature of an EI state.

The many-body trial wave function for the two-component plasma phase is a direct generalization of that for the one-component model:

$$\Psi_{2cp}=e^{\Sigma_{i\neq j}u(\mathbf{r}_{i,e}-\mathbf{r}_{j,e})}e^{\Sigma_{i\neq j}u(\mathbf{r}_{i,h}-\mathbf{r}_{j,h})} \times e^{\Sigma_{i,j}v(\mathbf{r}_{i,e}-\mathbf{r}_{j,h})}D_{e\uparrow}D_{e\downarrow}D_{h\uparrow}D_{h\downarrow}, \tag{2}$$

where the D's are the Slater determinants, composed of plane waves, filled up to a closed-shell momentum state in calculations using periodic boundary conditions. The Jastrow factors u and v are in the form of

$$u(\mathbf{r})=\frac{A}{r}(1-e^{-r/F})+c_u e^{-(r/r_u)^2} \tag{3}$$

and

$$v(\mathbf{r})=-\frac{A}{r}(1-e^{-r/F})+c_v e^{-(r/r_v)^2}. \tag{4}$$

A, F, c_u, c_v, r_u, and r_v are all variational parameters.

For the EI phase, the wave function is written in the explicit pairing form as[15,19]

$$\Psi_{ex}=e^{\Sigma_{i\neq j}u(\mathbf{r}_{i,e}-\mathbf{r}_{j,e})}e^{\Sigma_{i\neq j}u(\mathbf{r}_{i,h}-\mathbf{r}_{j,h})} \times e^{\Sigma_{i,j}v'(\mathbf{r}_{i,e}-\mathbf{r}_{j,h})}D_{eh}^{(1)}D_{eh}^{(2)}, \tag{5}$$

where D_{eh} is

$$D_{eh}=\begin{vmatrix} f(\mathbf{r}_{1,e}-\mathbf{r}_{1,h}), & \ldots, & f(\mathbf{r}_{1,e}-\mathbf{r}_{N,h}) \\ \cdot & & \cdot \\ \cdot & & \cdot \\ \cdot & & \cdot \\ f(\mathbf{r}_{N,e}-\mathbf{r}_{1,h}), & \ldots, & f(\mathbf{r}_{N,e}-\mathbf{r}_{N,h}) \end{vmatrix}, \tag{6}$$

and the superscripts $(1)=(\uparrow,\downarrow)$, $(2)=(\downarrow,\uparrow)$ refer to the spin of electron and hole.[20] The pairing wave function $f(\mathbf{r}_{i,e}-\mathbf{r}_{j,h})$ is taken as

$$f(\mathbf{r}): e^{-r/R_{ex}}$$

or

$$e^{-(r/R_G)^2}, \tag{7}$$

where R_{ex} (or R_G) is another variational parameter. Systematically better choices for $f(\mathbf{r})$ can be made, a point to which we shall return at the end of this paper.

In our variational calculations, we first optimize A which was found to deviate from that given by the plasmon condition for the two-component system.[21] The optimal F's are found to be given by the cusp-conditions[21]. When the exponential form is used for the pairing wave function in the EI, we must reduce the sharpness of the cusp-condition $dv'/dr|_{r=0}$ in $v'(\mathbf{r})$ by $1/R_{ex}$. For $r_s=2$ in the EI, the Gaussian pairing wave function yields a slightly lower energy. For $r_s=3$ and larger, the exponential form is lower in energy, although the Gaussian form with the appropriate cusp-conditions in the Jastrow factors is always very close. We then fix the values of A, F, R_{ex} (or R_G), and introduce the additional variational parameters c_u, c_v, r_u, and r_v to further optimize the energy. They yield an additional $\sim$ 5% lowering in energy at $r_s=2$.

Our results for the total energy are summarized in Fig. 1. We first make a few qualitative observations. With the VMC method, the energy of the 2CP has a minimum at $r_s\sim 2$, in agreement with previous work.[8,3,14] At $r_s=2$, the 2CP energy is $E_{r_s=2}=-0.90$ Ry, higher than that of a single exciton -1 Ry. It rises sharply on the lower r_s, higher density side due to the rise of the kinetic energy, and rises much more slowly on the larger r_s, lower density side. We are unable to resolve if there is a second minimum at a larger r_s, and this remains an important question to be answered.[2] Within the range of r_s investigated, which is between $r_s=2$ and $r_s=10$, the energy of the EI decreases slowly and monotonically with increasing r_s, approaching the isolated exciton value. At $r_s=2$, we find $E_{ex}=-0.95$ Ry, which is lower than that of the 2CP at the same density. Although the minimized energy of the EI changes relatively little with r_s, the optimal variational parameters change significantly, with the typical size of a single pair, i.e., the optimal value of R_{ex} or R_G, increasing with decreasing r_s.

For the present model system, the two-component plasma phase always has a weak excitonic instability due to the perfect nesting of the Fermi surfaces of the electrons and holes. The effects on total energy due to such Fermi-surface instability have been estimated by Brinkman and Rice.[22] This effect is also captured in the HF theory of Comte and

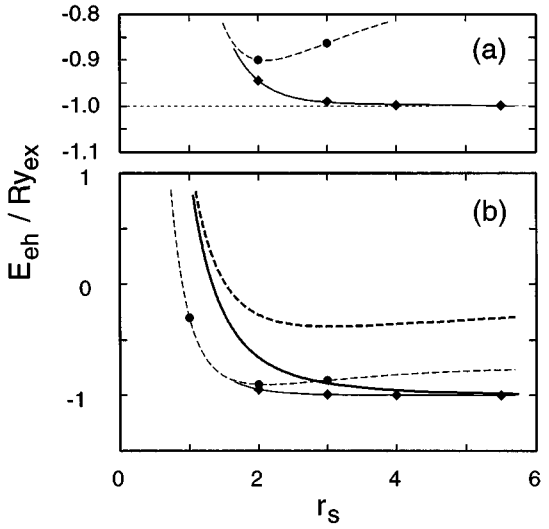

FIG. 1. Comparison of the total energy for the two-component plasma phase (dashed lines) and the excitonic insulator phase (solid lines) as a function of the density parameter r_s. The heavy lines indicate the mean field calculations while the solid symbols are calculated within the VMC approach. Part (a) shows an expanded scale.

Nozières,[5] and our evaluation of the ground state energy for this approximation is also shown in Fig. 1.[17,18] The regime of weak (i.e., exponential in coupling constant) instability is in the high density (small r_s) regime. For $r_s \sim 2$ the EI phase is already one of strong pairing. Our VMC introduces the correlation effects in the 2CP and EI phases on an equal footing. These are quantitatively important and determine the substantial stabilization of the EI phase at this relatively high density.

The finite size effects are large, particularly in the two-component plasma phase. We show in Table I the size dependence of the total energies of both the 2CP and the EI phases at $r_s=2$. The extrapolation to the thermodynamic limit is done following the approach of Tanatar and Ceperley[23] for the 2CP:

$$E_{\rm inf}=E_N+b_1(r_s)\Delta T_N+b_2(r_s)/N. \tag{8}$$

Here E_N is the calculated energy for N electron-hole pairs, ΔT_N is the correction for the noninteracting system, and the fitting coefficients depend on r_s. We estimate the uncertainty in the extrapolation procedure to be roughly 0.002 Ry. For the EI phase, the energy is essentially converged within the range of N studied. It is clear that the energy difference between the two phases is well beyond the remaining uncertainties from the finite size effects.

TABLE I. Finite size effects for the total energies of an equal-mass, electron-hole system at $r_s=2$ for both the two-component plasma phase and the excitonic insulating phase. Energies are in exciton Rydbergs, and the particle number per spin is given separately in the parentheses.

Particle number	2CP (Ryd)	EI (Ryd)
(27 27)	−0.935	−0.957
(33 33)	−0.912	−0.955
(57 57)	−0.894	−0.951
(81 81)	−0.917	−0.946
(93 93)	−0.906	−0.946
∞	−0.900(2)	−0.946

TABLE II. Comparison of correlation energies (in exciton Rydbergs) from various methods at several values of r_s for the two-component plasma phase.

r_s	HA[b]	RPA[b]	PSC[a]	FSC[a]	HNC[c]	VMC
0.5					−0.93	−0.87
1.0	−0.69	−0.76	−0.76	−0.74	−0.71	−0.68
2.0	−0.50	−0.55	−0.64	−0.62	−0.56	−0.54
3.0	−0.41	−0.45	−0.59	−0.55		−0.50

[a]Reference 8.
[b]Reference 3.
[c]Reference 14.

We now compare the variational Monte Carlo results to previous work for the two-component plasma phase and assess the resulting differences. In Table II, we compare the correlation energies at several densities. These are calculated by subtracting from the total energy the Hartree-Fock energy per pair, given by

$$E_{\rm HF}=\frac{3}{5}\left(\frac{9\pi}{4}\right)^{2/3}\Big/r_s^2-\frac{3}{\pi}\left(\frac{9\pi}{4}\right)^{1/3}\Big/r_s, \tag{9}$$

in exciton Rydbergs. The VMC results agree quite well with the HNC method, but there is no consistently good agreement with other methods. The FSC and the PSC give the lowest energies, with the latter being still lower than the single exciton energy. It should be stressed that the FSC and PSC calculations are not variational, and may overestimate the binding energy.

The comparison of total energies shows the quantitative difference between the present nonperturbative and the previous, mostly perturbative, methods. Qualitative information is available through differences which appear in the pair-correlation functions. The pair correlation function $g(\mathbf{r}_1,\mathbf{r}_2)$ is

$$g(\mathbf{r}_1,\mathbf{r}_2)n^2=2N(2N-1)\langle\rho(\mathbf{r}_1)\rho(\mathbf{r}_2)\rangle. \tag{10}$$

N is the total number of electrons, or holes, per spin. For the electron-hole correlation function, the prefactor $2N(2N-1)$ on the right-hand side should be replaced by $(2N)^2$. In Fig. 2, we show the electron-electron correlation functions for the 2CP phase calculated in the RPA,[8] FSC,[8] and HNC (Ref. 14) approximations, in comparison with the present VMC results, for $r_s=2$. The RPA yields negative results at small distances, similar to its failure in the one-component system. The FSC corrects this error, but exhibits very large oscillations, especially at distances shorter than the exciton Bohr radius which is unphysical. In contrast, VMC gives an essentially monotonic function, with Friedel oscillation amplitudes which are too small to be seen on this scale at $r_s=2$. The pair correlation functions found in the HNC approximation,[14] also illustrated in Fig. 2, are in good agreement with the present VMC results.

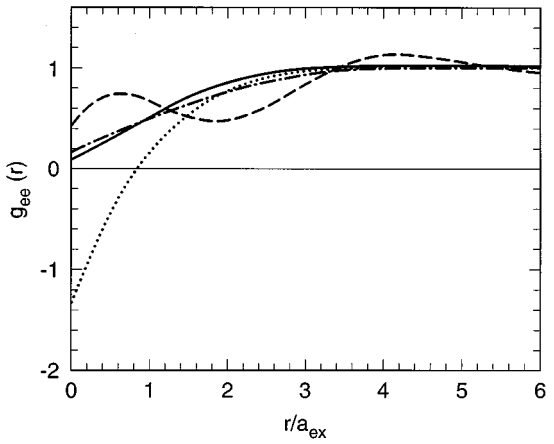

FIG. 2. Electron-electron pair distribution function for the two-component plasma at $r_s=2.0$ from RPA (dotted line), FSC (dashed line), HNC (Ref. 14) (dash-dot line), and from the VMC (solid line).

Some insight into the stabilization of the EI is given by the pair correlation functions. For $r_s=2$, these are compared in Fig. 3. The explicit pairing incorporated in the wave function of Eq. (5) through $f(\mathbf{r}_e-\mathbf{r}_h)$ dramatically increases the short range electron-hole correlation out to the range of approximately an exciton Bohr radius as expected. In fact, the shape and magnitude of $g_{eh}(r)$ are quite similar to expectations based on the correlation function evaluated in the limit of a dilute exciton gas:

$$g_{eh}(r)=\frac{4}{3}r_s^3 e^{-2r/a_{ex}}+1. \tag{11}$$

This is also shown in Fig. 3(a), for comparison. The close agreement is indicative of the strong pairing character of the state even at $r_s=2$. These short range correlations lower the energy. Since they are already incorporated at the mean field level, the mean field energy for the EI phase is substantially lower than the HF result for the 2CP, as seen in Fig. 1. These short range electron-hole correlations impede the electron-electron short range repulsion generated by correlation effects, as seen in Fig. 3(b). The balance favors the excitonic correlations.

Figure 4 shows both the electron-electron and the electron-hole pair distribution functions for the 2CP phase at $r_s=0.5$, calculated with the VMC method. The $g_{eh}(r)$ at $r=0$ shows a factor of 1.8 enhancement over the noninteracting value even at such a high density. The value of $g_{eh}(r=0)$ is a measure of the correlation-induced enhancement of the luminescence rate τ^{-1}. For non-k-conserving optical transitions $\tau^{-1}/\tau_o^{-1}=g_{eh}(r=0)$, where τ_0^{-1} is the spontaneous emission rate in the absence of interactions.[1] For k-conserving transitions, the necessary correlation function is somewhat different and less intuitive. Nevertheless, $g_{eh}(r=0)$ should still be indicative of the relative importance of excitonic correlations. The results in Fig. 4 indicate the importance of electron-hole correlations, even at rather high densities.

In Fig. 5, we show the calculated $g_{eh}(r)$ in the 2CP phase for the range of densities studied. The degree of short range electron-hole correlation changes dramatically with density

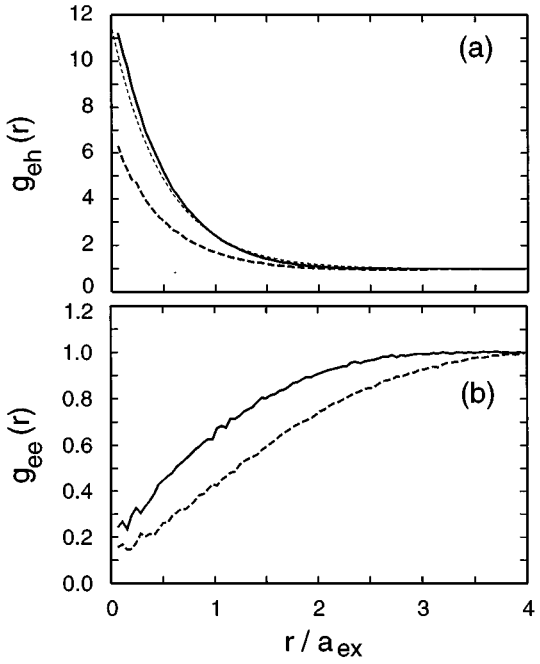

FIG. 3. Electron-electron (b) and electron-hole (a) pair distribution functions for the two-component plasma (dashed lines) and the excitonic insulator (solid lines) phases at $r_s=2.0$ from the VMC. The distribution function derived assuming a dilute exciton gas is shown in part (a) for reference (short dashed line)

over this range. The value of $g_{eh}(r=0)$ must be obtained by extrapolation, which has increased uncertainties for larger r_s. Nevertheless, the rapid increase at large r_s is as expected; for a dilute exciton gas $g_{eh}(r=0)=(4/3)r_s^3$ Our VMC estimate of $g_{eh}(r=0)$ is compared to other theories in the inset. We find the best overall agreement with HNC calculations. It is noteworthy that the HA underestimates the excitonic correlations. The HA is most closely related to the many-body treatments most widely applied to study spectra and material gain in semiconductors.[1,6] Recall that the relevant density range for semiconductor lasers is typically $r_s<0.5$. While the RPA or HA underestimate the correlations, this is a regime in which the density dependence of those correlations is relatively weak.

Before closing, we note that a conceptually more appealing choice of the pairing wave function can be made by use of the BCS-like mean-field theory of the excitonic phase for the pairing wave function f in Eq. (7).[5] The complete numerical solution to the resultant coupled-equations that one encounters in the mean-field theory is straightforward.[17,18] Qualitatively, the result in the low density limit approaches the exponential form in Eq. (7). In the high density limit, the pairing wave function approaches a Fermi function (in k space) and smoothly approaches the 2CP case. This continuous evolution from the EI to the 2CP is mimicked in our simple form [Eq. (7)] by an increase in R_{ex} or R_G as r_s decreases. It is also consistent with our finding that an exponential form gives a slightly lower energy in the EI phase for lower density while for $r_s=2$ the Gaussian form is better. For the gross quantities studied in this paper, our simple variational ansatz with exponential or Gaussian should suf-

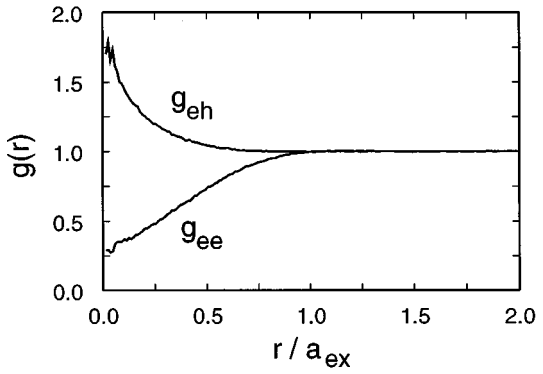

FIG. 4. Electron-electron (lower curve) and electron-hole (upper curve) distribution functions for the two-component plasma at $r_s = 0.5$ from the VMC.

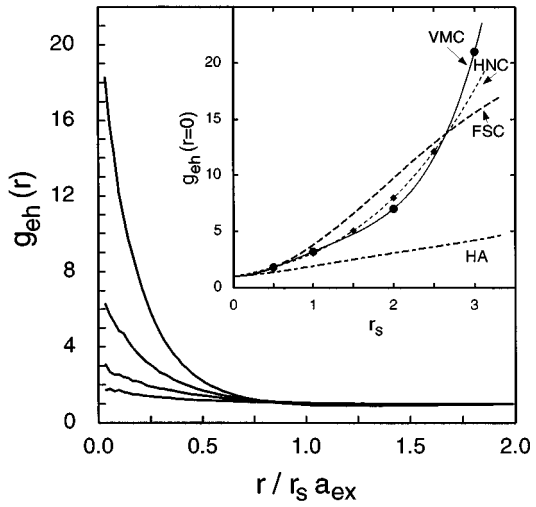

FIG. 5. Calculated electron-hole pair distribution function for the two-component plasma phase for $r_s = 0.5$, 1.0, 2.0, and 3.0. Inset: g_{eh} at zero separation as a function of r_s, from the RPA (Ref. 8), from the FSC (Ref. 8), from the HNC (Ref. 14), and from the present VMC.

fice. However, the incorporation of a better approximation to the pairing wave function, e.g., from the mean-field solution for the EI, in the VMC calculations might lower the energy for the intermediate density regime. One should note that the mean-field solution allows for no extra variational parameters in the pairing wave function. The screening effect (equivalent physically to the variation in R_{ex}) could be incorporated phenomenologically through a screened Coulomb interaction in the mean-field equations. Also, other effects such as band anisotropy and nonparabolicity can be readily incorporated into the mean-field theory.

To summarize, we have studied the model system of an equal mass, electron-hole system with a variational Monte Carlo approach. Ground state total energies for both the two-component plasma phase and the excitonic insulating phase have been calculated on an equal footing. The energy and the pair-correlation functions of the 2CP phase found in the present calculations differ significantly from those found in the random-phase approximation and self-consistent local-field approaches. The Mott criterion for the metal-insulator transition does not apply to the two-component system. The EI phase is found to be lower in energy over the whole range of density.

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