Path integral Monte Carlo results for Bose condensation of mesoscopic indirect excitons

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First principle results for small clusters of strongly correlated indirect excitons in a harmonic confinement potential are presented. At low temperature Bose condensation is verified. The condensate fraction and the superfluid density are computed. The importance of a correct treatment of the Fermi statistics of electrons and holes is demonstrated.

1 Introduction Over the last three decades systems of spatially separated ("indirect") excitons [1] have attracted increasing attention due to their increased life time allowing the excitons to reach a quasi-equlibrium state. In recent years, indirect excitons have been experimentally realized by several groups, e.g. [2, 3], for recent theoretical results for electrical field induced separation of electrons and holes, cf. refs. [4, 5]. Among the most exciting and still highly disputed questions is the possibility of Bose Einstein condensation (BEC) of indirect excitons in these systems. To achieve a conclusive proof of BEC is not only experimentally challenging, but also theoretically difficult. The main challenge here is that the predictions should not depend on approximations, such as the assumption of Bose statistics of individual excitons.

In this paper, we present first-principle results where electrons and holes are treated accurately as Fermi particles. For comparison, we also provide results from a "bosonic model". We will not use a simple pair approximation which replaces N indirect electron hole pairs by N excitons residing in a single layer. The reason is that we have found that the results of this frequently used model are very sensitive to the used exciton-exciton interaction, which in fact is very different from a simple dipole interaction, see e.g. [5]. In order to focus on the effect of Fermi vs. Bose statistics, we consider as reference case the same two layer systems of electrons and holes (with the exact two-particle interactions) but in the N-particle density matrix (or wave function) restrict ourselves to symmetric permutations, i.e. any permutation of electrons is accompanied by the same permutation of holes.

2 Model The Hamiltonian of the system of $N_e = N_h = N$ indirect electron-hole pairs reads

$$\hat{H} = \hat{H}_e + \hat{H}_h + \sum_{i=1}^{N}\sum_{j=i+1}^{N} \frac{e_i e_j}{\varepsilon|\mathbf{r}_i - \mathbf{r}_j|}, \quad \hat{H}_a = \sum_{i=1}^{N_a}\left(-\frac{\hbar^2}{2m_a^*}\nabla^2_{\mathbf{r}_i} + \frac{m_a^*}{2}\omega_a^2 r_i^2\right) \tag{1}$$

where $a = e, h$, electrons and holes are located in two layers separated by a distance d and interlayer tunneling is assumed negligible. Below, all lenghts will be given in units of the effective Bohr radius $a_B = \hbar^2\epsilon/m_e^* e^2$, and we use ZnSe parameters with $m_h^*/m_e^* = 2.47$ and $\epsilon = 8.7$ (this results in $a_B = 3.07$ nm). The density is controlled by the trap frequency (we use $m_e^*\omega_e^2 = m_h^*\omega_h^2$) and characterized by the coupling

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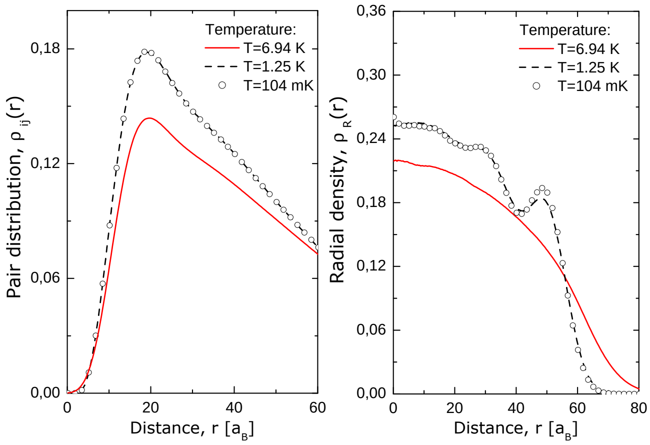

Fig. 1 Pair distribution (a) and Radial density distribution (b) of 30 trapped excitons at strong coupling, $\lambda = 15$ for three temperatures. Results of the bosonic model.

parameter $\lambda = (e^2/\epsilon l_0)/(\hbar\omega_e)$ with $l_0^2 = \hbar/m_e^*\omega_e$. The properties of the system of N electrons and holes at a finite temperature T are determined by the canonical density operator $\hat{\rho} = \exp[-\hat{H}/k_BT]/Z$. Due to the Fermi statistics $\hat{\rho}$ has to be antisymmetric with respect to arbitrary electron and hole exchanges separately, i.e. it contains a sum of $N_e! \times N_h!$ contributions, e.g. [8]. This exact procedure is carried out in the fermionic calculations below. Our reference case ("bosonic model", see above) contains, instead, only $N!$ contributions of pairwise identical electron and hole permutations.

The full density operator is evaluated exactly using the path integral Monte Carlo (PIMC) technique. In order to obtain an accurate treatment of the BEC in this system, no further simplifications (such as fixed node approximations) are performed. This presently restricts our fermionic calculations to about 10 particles and the temperature to values above approximately $10^{-4}Ha$ (Ha denotes the Hartee energy, with $Ha = 53.93$ meV for ZnSe) due to the Fermion sign problem. In contrast, the bosonic calculations have no such limitations. To investigate the excitonic systems in the temperature range from 100 mK to several Kelvin the number of time slices in the path integral Monte Carlo was varied $m = 100 - 600$. Details of the simulations are given in ref. [8].

3 Results of the bosonic model. To reduce the space of parameters, in this paper we concentrate on the region of strong Coulomb coupling, choosing λ in the range of $18 > \lambda > 10$. Further, the interlayer distance is kept fixed to a value of $d = 6.65a_B$, which corresponds to the induced dipole moment of the indirect excitons in 30.7 nm wide ZnSe quantum well subjected to the electric field of 20 kV/cm applied normal to the QW plane [5].

Consider first the spatial arrangement of the excitons in the trap. Due to the electron and hole charge the excitons can be strongly correlated. This is seen for the case of $N = 30$ pairs at the coupling parameter $\lambda = 15$ in Fig. 1. With the reduction of temperature, the initially homogeneous radial distribution develops a shell structure which is a precurser of a strongly localized crystal-like state which occurs in electron and exciton systems [6, 7] at still lower density.

Let us now consider the quantum statistical properties of the excitons. The permutation sum of the density operator contains cycles of length (i.e. involving) one to N (identical particles). In a classical system, only the identity permutation occurs, whereas in the limit of zero temperature, an ideal quantum gas has equal probability of all permutations. Fig. 2a shows the simulation results for the probability $P(L)$ of cycles of length L for 20 particles and various temperatures. The calculation results are for a strongly interacting system ($\lambda = 15$) but nevertheless clearly confirm this trend. The length of the plateau of the

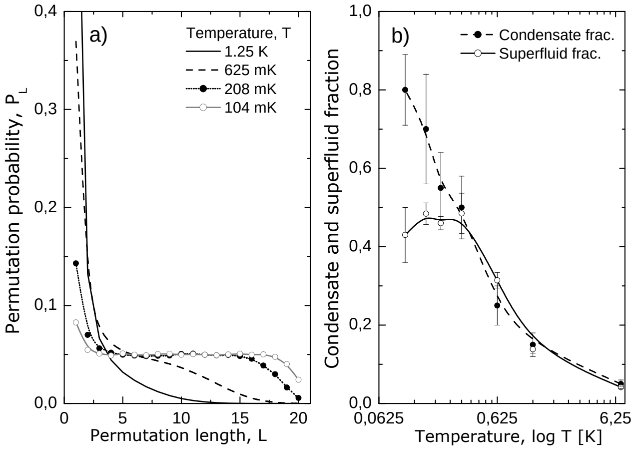

Fig. 2 **a**: Distribution of permutation cycles for four temperatures. **b**: Fraction of Bose condensed and of superfluid excitons for a total of $N = 20$ trapped electron hole pairs at strong coupling, $\lambda = 15$. Results of the bosonic model.

curve $P(L)$ can be used to compute the number of particles in the Bose condensate, e.g. [9]. Using the threshold value $P_L(L; N_{e(h)}) = 0.8/N_{e(h)}$ we obtain the condensate fraction, Fig. 2b which reaches more than 80% at low temperatures.

The next interesting quantity is the fraction of the superfluid (mass) density $\gamma_s = \rho_s/\rho$ of excitons which, within the two-fluid model is computed from the classical and quantum moment of inertia, I_c and I_q according to $\gamma_s = 1 - I_q/I_c$. The quantities I_c and I_q are effectively computed in PIMC simulations from the area enclosed by the particle pathes $\mathbf{A}$, using the Eq. $\rho_s/\rho = 4m^2\langle A_z^2\rangle/\hbar^2\beta\langle I_z\rangle$, e.g. [9]. The numerical results are shown by the solid line in Fig. 2b

4 Fermionic results. Let us now consider the results of the exact fermionic calculations. Fig. 3 shows results for $N = 6$ electron hole pairs at the temperature $T = 312\mathrm{mK}$. Part **a** shows the effect of the Fermi statistics on the radial distribution (RDF) of the electrons. Clearly the Fermi repulsion between two electrons (and, analogously, two holes) favors an increased localization of individual particles. This is seen, in particular, from the increased localization of the center particle (five particles form a spherical shell) and from the slightly reduced density inbetween the center particle and the shell. Although this difference between Fermi and Bose statistics results for the spatial distribution of the particles appears to be small, it has a large effect on the superfluid fraction, cf. Fig. 3b. At low in-layer density (large λ), both results agree within the statistical errors. This is readily understood, since at large coupling where the wave function overlap is small, correlation effects due to the Coulomb repulsion are much stronger than quantum exchange effects. However, above a critical value of $\lambda \approx 15$, the differences of the two calculation grow rapidly. While the bosonic model exhibits a continuous growth of the superfluid fraction γ_s, the exact calculation reveals a monotonous reduction of γ_s for smaller values of λ. Obviously, at these higher densities the relevance of Coulomb correlations decreases compared to the Fermi repulsion (exchange) of two adjacent electrons or holes. Thus the trend seen in Fig. 3a is growing further: the Fermi statistics reduces the overlap of two electrons (two holes) compared to a Bosonic model. As a consequence, the exciton superfluid fraction decreases.

5 Discussion. In summary, we have presented first principle path integral Monte Carlo results for indirect excitons confined in a harmonic trap. The simulations concentrated on the region of strong Coulomb coupling, i.e. low temperatures and comparatively low in-layer density of electrons and holes. From our previous investigations [6, 7] we know that this parameter range corresponds to the co-called Wigner

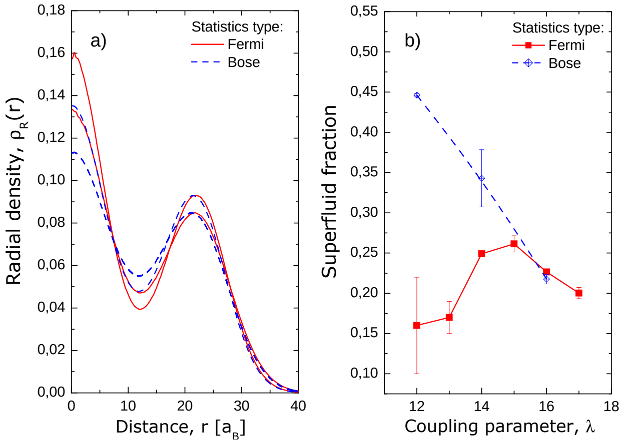

Fig. 3 Comparison of the Bose model and the exact fermionic simulation for 6 electron-hole pairs. **a**: Radial density distributions of electrons (lower curves) and holes (upper curves) for $\lambda = 14$. **b**: Superfluid exciton fraction versus coupling strength at $T = 312\mathrm{mK}$.

molecule state which is similar to Fermi liquid behavior in a macroscopic system. This behavior is found also in the present simulations, in particular in the radial and pair distributions of electrons and holes in their respective layers. However, due to the strong interlayer correlations resulting in formation of tightly bound indirect excitons, the present system shows, in addition, strong bosonic many-particle features. To analyze the latter, we have computed the fraction of Bose condensed excitons as well as the superfluid fraction of excitons and observed remarkably large values.

The present system of electron-hole pairs if frequently modeled by a single layer systems of excitons which are treated as bosons. In our simulations, we were able to test this model against the exact two-component fermion system in the given parameter range. We have found that the bosonic model works well at strong Coulomb coupling, i.e. for $\lambda > 15$. However, for smaller values of the coupling parameter, the bosonic model yields qualitatively wrong results for the superfluid fraction and is not applicable. On the other hand, we expect that the results for the condensate fraction will be less drastically affected by the choice of the model.

Finally, we mention that the present system of strongly coupled indirect excitons is expected to exhibit another striking quantum many-particle phenomenon – the formation of a supersolid which was predicted by Andreev and Lifshitz [10], Leggett [11] and others and which was recently observed in helium [12]. The present system of excitons exhibits crystallization at slightly larger values of λ than presented here. Preliminary results indicate that even at these parameters, there will remain a finite superfluid fraction of excitons.

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