Superfluidity of indirect excitons in a quantum dot.

Yu.E. Lozovik\textsuperscript{a}, S.A. Verzakov\textsuperscript{a}, and M. Willander\textsuperscript{b}

\textsuperscript{a}Institute of Spectroscopy, Russian Academy of Sciences, 142092 Troitsk, Moscow region, Russia

\textsuperscript{b}Göteborg University, Chalmers University of Technology, S-41296, Göteborg, Sweden

The superfluidity and Bose-Einstein condensation of indirect excitons in two-dimensional quantum dot are studied by path-integral Monte Carlo simulations. The temperature dependence of superfluid and Bose-condensed fraction are calculated at different strengths of interaction. Using the Kosterlitz-Thouless recursion relations, we also predict behavior of superfluid fraction in macroscopic large systems.

PACS number(s): 71.35.Lk, 36.40.Ei, 74.80.-g, 02.70.Lq

I. INTRODUCTION

Low-dimensional electron-hole systems in semiconductor heterostructures, quantum dots and quantum wires are of increasing experimental and theoretical attention now. Conceptually new physical effects can take place in these systems.\textsuperscript{1,2} One of the most interesting examples of systems considered is the structure that consists of two vertically connected two-dimensional quantum wells. Under the action of laser radiation, each well is occupied by carriers of different types, which form a two-layered electron-hole system. As has been shown in Ref.\textsuperscript{3}, superfluidity of indirect excitons, which are bounded states of pairs of spatially-separated electrons and holes, can appear in the system and manifests itself as persistent electric currents in each two-dimensional layer. The behavior of phase diagram in strong magnetic field\textsuperscript{4} and Josephson effects\textsuperscript{5} have been also studied. A number of interesting experiments for magnetoexcitons with spatially-separated carriers in coupled quantum wells have been recently carried out.\textsuperscript{6-8}

The surface roughness can lead to the excitons localization\textsuperscript{9} and thus it behaves like a
natural quantum dot. Excitons can also be confined in vertically coupled artificial quantum dots. Hence, the investigation of "lakes" of excitons is essential.

The goal of this article is to study the onset of the superfluidity of indirect excitons in two-dimensional (2D) quantum dot. In a 2D system at low densities \( n \ll a^{-2} \) (\( a \) is exciton radius), potential barrier that is generated by dipole-dipole repulsion of indirect excitons suppress exchanges of constituent particles, electrons and holes. Therefore the system of 2D indirect excitons at low density can be treated as Bose system. (Other situations in which excitons can be assumed to be bosons were discussed in Refs. [11][13].) Moreover, under the same conditions indirect excitons can be thought of as point-like particles with unidirected dipole momenta. Another system which can be mapped onto this model is that of trapped Bose atoms with dipole momenta induced by d.c. electric field or standing electromagnetic wave in resonance with atomic transition. For the sake of definiteness we present explanation below in terms of excitonic cluster. In the absence of interaction between particles, we use a semi-analytical method based on a recursion relation for canonical partition functions. Clusters of interacting excitons are explored by the path-integral Monte Carlo technique.

The paper is organized as follows. In the next section the model and controlling dimensionless parameters are introduced. In Sec. II we outline the Monte Carlo technique and a semi-analytical approach. Sec. III is devoted to the discussion of the results.

II. THE MODEL HAMILTONIAN

As discussed above, we treat indirect exciton as a structureless boson with effective mass \( m \) and effective dipole moment \( d \) perpendicular to the plane of 2D quantum dot. The confining potential of the quantum dot we take in a harmonic form. Hence, the model Hamiltonian is given by

\[
\hat{H} = \sum_{i=1}^{N} \left[ -\frac{\hbar^2}{2m} \Delta_i + \frac{m\omega^2 |r_i^2|}{2} \right] + \sum_{i<j} \frac{d^2}{|r_{i,j}|^3}.
\]  (1)
Choosing as length unit $r_0 \equiv \sqrt{\hbar/m\omega}$, we introduce dimensionless controlling parameters for the system at the finite temperature $\beta^{-1}$: dimensionless temperature $T \equiv \beta^{-1}/(\hbar^2/(2mr_0^2))$ and interaction constant $k \equiv (|d|^2/r_0^3)/(\hbar^2/(2mr_0^2))$.

### III. SIMULATION METHODS AND CALCULATED PROPERTIES

The canonical ensemble of noninteracting Bose system ($k = 0$) can be studied with the help of simple semi-analytical procedure analogous to that has been used for particles in a harmonic trap interacted by a harmonic law. The method that has been used is based on universal connections between partition functions of canonical and grand canonical ensembles

$$Z(u) = \sum_N u^N Z_N,$$
$$u \equiv \exp(\beta \mu),$$
$$Z_N = \frac{1}{N!} \left. \frac{d^N}{du^N} Z(u) \right|_{u=0}. \quad (2)$$

Here $\mu$ is the chemical potential of the grand canonical ensemble and $N$ is the number of particles in the canonical ensembles. Starting from Eq. (2), one can derive a recursion relation for the canonical partition functions of a noninteracting Bose gas with an arbitrary one-particle spectrum $\varepsilon_i$:

$$Z_N(\beta) = \frac{1}{N} \sum_{n=0}^{N-1} Z_n(\beta) Z_1((N-n)\beta), \quad (3)$$

$$Z_0(\beta) = 1, \quad Z_1(\beta) = \sum_i \exp(-\beta \varepsilon_i).$$

Hence, the numerical procedure consists in calculations of the canonical one-particle partition functions at temperatures $T/N, 2T/N, \ldots, T$ and iterations of Eq. (3). Generalization of the Eq. (3) to the case of partition function derivatives, in form of which interesting thermodynamic averages (see this section below) can be presented, is obvious.

Cluster of interacting excitons has been studied by the path-integral Monte Carlo calculations (for comprehensive review of application the path-integral method to the Bose
systems see Ref. 16). This technique is based on the Trotter procedure as a result of which thermodynamic averages on $D$ dimensional quantum system are expressed via averages on $D + 1$ dimensional classical system, which is created by multiplication of the configuration space of the initial system along imaginary time direction. Calculated in so called primitive approximation, the potential energy of the effective classical system that corresponds to the quantum model with Hamiltonian (1) is

$$\beta V_{\text{eff}} = \frac{1}{PT} \sum_{p=0}^{P-1} \left( \sum_{i=1}^{N} \left[ \frac{|r_i^{(p+1)} - r_i^{(p)}|^2}{4/(PT)^2} + |r_i^{(p)}|^2 \right] + \sum_{i<j} k \frac{|r_i^{(p)} - r_j^{(p)}|^3}{|r_i^{(p)} - r_j^{(p)}|^3} \right),$$

where $P$ is the number of effective system layers, $N$ is the number of particles in one layer, which is equal to the number of particles in the original quantum system and $r_i^{(p)}$ stands for the 2D radius vector of $i$-th particle in the layer $p$. Bose statistics is taken into account by summation over particles permutations $\mathcal{P}$ during Monte Carlo simulation. The energy of the effective system depends on $\mathcal{P}$ by assumption $r_i^{(P)} = r_i^{(0)}$.

Our attention has been focused on superfluid properties of excitons. One of the most dramatic manifestations of the superfluidity is the deviation of the effective moment of inertia from its rigid or "classical” value $I_{cl} \equiv \langle \sum_{i=1}^{N} m_i r_i^2 \rangle$. By definition, the effective moment of inertia is the linear response function to a uniform rotation field with angular frequency $\Omega$

$$I_{eff} \equiv \frac{\partial}{\partial \Omega} \left. \text{tr} \left\{ L_z \exp(-\beta (H - \Omega L_z)) \right\} \right|_{\Omega=0} = \beta \langle L_z^2 \rangle.$$

Only the normal fluid gives rise to the $I_{eff}$. Thus, the superfluid fraction of the cluster is

$$\nu_s \equiv \frac{n_s}{n} = \frac{I_{cl} - I_{eff}}{I_{cl}}.$$

In order to calculate $\nu_s$ in case of ideal gas in a trap (i.e. at $k = 0$, see definition of $k$ near Eq. (4)) by using above mentioned recurrent procedure, firstly, one should express $I_{eff}$ and $I_{cl}$ in form of partition function derivatives

$$I_{eff} \equiv \beta \langle L_z^2 \rangle = \frac{1}{\beta Z} \frac{\partial^2}{\partial \Omega^2} Z_{\Omega=0},$$

$$I_{cl} \equiv \langle \sum_i m_i r_i^2 \rangle = \frac{1}{\beta \omega Z} \frac{\partial}{\partial \omega} Z.$$
Here $Z^\Omega \equiv tr \{ \exp(-\beta(\hat{H} - \Omega \hat{L}_z)) \}$ is the partition function of the system rotating with the frequency $\Omega$, $Z \equiv Z^{\Omega=0}$ is the partition function of the system at rest. Secondly, explicit expression for one-particle partition function $Z^\Omega$ is needed. The spectrum of the Hamiltonian $\hat{H}^\Omega = \hat{H} - \Omega \hat{L}_z$ at $k = 0$ is $\varepsilon_{n,m} = \hbar \omega (2n + |m| + 1) - \hbar \Omega n$, where $n = 0, 1, \ldots$ and $m = 0, \pm 1, \pm 2, \ldots$ are radial and angular quantum numbers ($\hbar m$ is the eigenvalue of the operator $\hat{L}_z$). After some algebra, one can write

$$Z^\Omega_1(\beta) = [4 \sinh(\hbar \beta (\omega - \Omega)/2) \sinh(\hbar \beta (\omega + \Omega)/2)]^{-1}$$

Calculation of superfluid fraction in case of $k \neq 0$ has been performed by path-integral Monte Carlo simulations. Applying the Trotter procedure to the quantum-statistics averages by which $I_{cl}$ and $I_{eff}$ are defined, one takes\(^\text{16}\)

$$I_{eff} = \frac{1}{P} \left\langle \sum_{i=1}^N \sum_{p=0}^{P-1} r_i^{(p)} \cdot r_i^{(p+1)} \right\rangle_p - 2T \left\langle |A|^2 \right\rangle_p$$

$$A = \frac{1}{2} \sum_{i=1}^N \sum_{p=0}^{P-1} r_i^{(p)} \times r_i^{(p+1)}$$

$$I_{cl} = \frac{1}{P} \left\langle \sum_{i=1}^N \sum_{p=0}^{P-1} r_i^{(p)} \cdot r_i^{(p)} \right\rangle_p$$

Here averagings are performed on the effective classical system, the moments $I_{cl}$ and $I_{eff}$ are measured in units of $m r_0^2 = \hbar / \omega$.

The fraction of Bose-condensed particles we calculate by the method introduced in Ref.\(^\text{18}\): the maximum length of permutation cycle in path-integral Monte Carlo simulation which has a nonzero probability is the number of particles in the condensate.

**IV. DISCUSSION OF THE SIMULATION RESULTS**

Calculated temperature dependencies of superfluid fraction are shown in Fig. 1. One can see superfluidity suppression induced by interaction at a fixed dot angular
frequency. Condensate depletion is obvious too (see Fig. 2). However after defining “average density” \( n \equiv N/(2\pi < r^2 >) \) and plotting \( \nu_s \) vs. dimensionless temperature \( \alpha \equiv m/(\beta \hbar^2 n) = 2\pi I_{cl}/(\beta \hbar^2 N^2) \), i.e. at a fixed density, one can see (Fig. 3) some rising of the superfluid fraction with interaction. But interaction, of course, depletes condensate even at fixed density (Fig. 4).

The investigated system is fully analogous to the atoms in a plane harmonic trap. BEC occurs for noninteracting system in two-dimensional harmonic trap in thermodynamic limit (contrary to the situation in homogeneous systems). For systems with repulsive interaction there is only some critical temperatures of transition to the new state without condensate (see Ref. [19 and references therein]).

Assuming Kosterlitz-Thouless (KT) scenario, we have estimated the critical temperature of the phase transition. Nonanalytic behavior of the free energy of the system and consequently a phase transition can be observed only in macroscopic systems. But in a computer simulation one deals with finite systems. Hence, the extrapolating procedure is necessary. We define thermodynamic limit as \( \omega \to 0, N \to \infty \) at \( n \equiv N/(2\pi < r^2 >) = \text{constant} \). In case of weak interaction this definition coincides with requirement \( N\omega^2 = \text{constant} \).

The extrapolation procedure (see Ref. [20] is based on mapping of a 2D system of vortices to the 2D logarithmic gas, which has KT transition.\(^{21,22}\)

The temperature of this gas, which is expressed in units of square of logarithmic gas charge, is \( T_{cg} = m/(2\pi \hbar^2 n\beta) = \alpha/(2\pi) \), the chemical potential (in the same units) is \( \mu = -T_{cg}\beta E_c \), where \( E_c \) is the vortex core energy in superfluid, and dielectric constant is \( \varepsilon = 1/\nu_s \). Kosterlitz-Thouless recursion relations lead to the universal jump of \( 1/(T_c \varepsilon) \) from 4 to 0 at the transition temperature. But in the finite systems superfluid vanishes smoothly enough (Figs. 1, 3). Such type of behavior can be analytically accounted by integrating recursion relations up to size of system (not to infinity).\(^{44}\)

The parameters of curve \( \nu_s(T_{cg}) \) are vortex core energy and diameter, which are defined by fitting analytic approximation to the Monte Carlo results. Then full integration of Kosterlitz-Thouless relations at fixed vortex core energy and core diameter gives critical value of
temperature.

Scaling results for different values of interaction constant $k$ gives, e.g., $\alpha_{KT}(0.1) = 0.92$, $\alpha_{KT}(1) = 1.19$.

ACKNOWLEDGMENTS

We wish to thank A.I. Belousov for fruitful discussion. The work has been supported by a grant from The Royal Swedish Academy of Science and INTAS.

* E-mail: lozovik@isan.troitsk.ru

1 T. Chakraborty and P. Pietilainen, *The Fractional Quantum Hall Effect* (Springer-Verlag, New York, 1988).

2 *Perspectives in Quantum Hall Effects*, edited by S. Das Sarma and A. Pinchuk, (John Wiley Publ., N.Y., 1997).

3 Yu.E. Lozovik and V.I. Yudson, Pisma ZhETF 22, 26 (1975) [JETP lett., 22, 26(1975)]; ZhETF, 71, 738 (1976) [JETP, 44, 389 (1976)]; Sol. St. Commun. 18, 628 (1976); 21, 211 (1977); Physica A 93, 493 (1978).

4 Yu.E. Lozovik and O.L. Berman, ZhETF 111, 5, 1879 (1997) [JETP 84, 5, 1027 (1997)]; Yu.E. Lozovik, O.L. Berman, and V.G. Tsvetus, Pisma ZhETF 66, 5, 332 (1997); Phys. Rev. B (in press).

5 Yu.E. Lozovik and A.V. Poushnov, Phys. Lett. A 228, 399 (1997).

6 A. Zrenner, L.V. Butov, M. Hang, G. Abstreiter, G. Bohm, and G. Weimann, Phys. Rev. Lett. 72, 3383 (1994); L.V. Butov, A. Zrenner, G. Abstreiter, G. Bohm, and G. Weimann, Phys. Rev. Lett. 73, 304 (1994).
7 M. Bayer, V.B. Timofeev, T. Gutbrod, A. Forchel, R. Steffen and S. Oshinno, Phys. Rev. B 52, R11623 (1995). M. Bayer, A. Schmidt, A. Forchel, F. Faller, T.L. Reinecke, P.A. Knipp, A.A. Dremin, and V.D. Kulakovskii, Phys. Rev. Lett. 74, 3439 (1995).

8 U. Sivan, P.M. Solomon and H. Strikman, Phys. Rev. Lett. 68, 1196 (1992).

9 G.S. Gevorkyan and Yu.E. Lozovik, Fiz. Tverd. Tela 27, 1800 (1985).

10 N.E. Kaputkina and Yu.E. Lozovik, Phys. Scr. 57, 541 (1998).

11 L.V. Keldysh and A.N. Kozlov, ZhETF 54, 978 (1968) [JETP 27, 521 (1968)].

12 C. Kallin and B.I. Halperin, Phys. Rev. B 30, 5655 (1984); Phys. Rev. B 31, 3635 (1985).

13 G. Vignale and A.H. MacDonald, Phys. Rev. Lett., 76, 2786 (1996).

14 F. Brosens, J.T. Devreese and L.F. Lemmens, Sol. St. Commun. 100, 123 (1996).

15 In case of Fermi statistics relation is

\[ Z_N(\beta) = \frac{1}{N} \sum_{n=0}^{N-1} \frac{1}{(-1)^{N-1-n}} Z_n(\beta) Z_1((N-n)\beta) \]

16 D.M. Ceperley, Rev. Mod. Phys. 67, 279 (1995).

17 G. Baym, in *Mathematical Methods in Solid State and Superfluid Theory*, edited by R.C. Clark and E.H. Derrick (Oliver and Boyd, Edinburgh, 1969), p. 121.

18 W. Krauth, Phys. Rev. Lett. 77, 3695 (1996).

19 W.J. Mullin, J. Low Temp. Phys. 106, 615 (1997); cond-mat/9610005; cond-mat/9709077.

20 D.M. Ceperley and E.L. Pollock, Phys. Rev. B 39, 2084 (1989).

21 J.M. Kosterlitz and D.J. Thouless, J. Phys. C6 1181 (1973).

22 P. Minnhagen, Rev. Mod. Phys. 59, 1001 (1987).
FIG. 1. Superfluid fraction \( \nu_s \) vs. dimensionless temperature \( T = 2/(\beta \hbar \omega) \) for excitonic cluster with number of particles \( N = 37 \): solid line \(- k = 0 \) (noninteracting case), solid triangles \(- k = 0.01 \), open circles \(- k = 0.1 \), solid circles \(- k = 1 \), open squares \(- k = 2.38 \), solid squares \(- k = 23.5 \), open triangle \(- k = 48.25 \).

FIG. 2. Condensed fraction \( \nu_0 \) vs. \( T = 2/(\beta \hbar \omega) \) for excitonic cluster with number of particles \( N = 37 \): solid line \(- k = 0 \) (noninteracting case), open circles \(- k = 0.1 \), solid circles \(- k = 1 \).

FIG. 3. Superfluid fraction \( \nu_s \) vs. \( \alpha = 2\pi I_{cl}/(\beta \hbar^2 N^2) \): solid line \(- k = 0 \) (noninteracting case), solid triangles \(- k = 0.01 \), open circles \(- k = 0.1 \), solid circles \(- k = 1 \), open squares \(- k = 2.38 \), solid squares \(- k = 23.5 \).

FIG. 4. Condensed fraction \( \nu_0 \) vs. \( \alpha = 2\pi I_{cl}/(\beta \hbar^2 N^2) \): solid line \(- k = 0 \) (noninteracting case), open circles \(- k = 0.1 \), solid circles \(- k = 1 \).
Fig. 1
Fig. 2
Fig. 3
