Sensitive linear response of an electron-hole superfluid in a periodic potential

Oleg L. Berman\textsuperscript{1,2}, Roman Ya. Kezerashvili\textsuperscript{1,2}, Yurii E. Lozovik\textsuperscript{3}, and Klaus Ziegler\textsuperscript{1,4}

\textsuperscript{1}Physics Department, New York City College of Technology, The City University of New York, Brooklyn, NY 11201, USA
\textsuperscript{2}The Graduate School and University Center, The City University of New York, New York, NY 10016, USA
\textsuperscript{3}Institute of Spectroscopy, Russian Academy of Sciences, 142190 Troitsk, Moscow, Russia
\textsuperscript{4}Institut für Physik, Universität Augsburg D-86135 Augsburg, Germany

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We consider excitons in a two-dimensional periodic potential and study the linear response of the excitonic superfluid to an electromagnetic wave at low and high densities. It turns out that the static structure factor for small wavevectors is very sensitive to a change of density and temperature. It is a consequence of the fact that thermal fluctuations play a crucial role at small wavevectors, since exchanging the order of the two limits, zero temperature and vanishing wavevector, leads to different results for the structure factor. This effect could be used for high accuracy measurements in the superfluid exciton phase, which might be realized by a gated electron-hole gas. The transition of the exciton system from the superfluid state to a non-superfluid state and its manifestation by light scattering are discussed.

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I. INTRODUCTION

A gas of excitons is a canonical example for an interacting many-body system \cite{1}. Excitons are bound states of an electron and a hole, which can be considered as a system with no effective electric charge. This justifies the assumption of a short-range interaction. The latter is caused by the Pauli principle because of the fermionic constituents. At low temperatures the excitons can form a superfluid as a collective many-body state. Moreover, in the presence of a periodic potential a Mott-insulating (MI) state is possible where the excitons form a state which is commensurate to the periodic structure of the potential minima. Both states, the superfluid and the MI phase, and the phase transition between them have been observed in an ultracold gas of bosonic rubidium atoms \cite{2}. Although it is more difficult to control the parameters of an exciton gas with present technologies, the similarity of the exciton gas and a bosonic gas of real atoms indicates that the formation of these two states and the phase transition between them should be accessible under proper experimental conditions.

Superfluidity in a two-dimensional (2D) system of electron-hole pairs was predicted on the basis of Cooper pairing within a BCS mean-field approach \cite{3} in Ref. \cite{4}. The BCS phase of electron-hole Cooper pairs in a dense electron-hole system and a dilute gas of indirect excitons, formed as bound states of electron-hole pairs, were also analyzed in coupled quantum wells (CQW) \cite{5,6}. This was followed by a number of detailed theoretical \cite{7-15} as well as experimental studies \cite{16-24}. Besides the superfluid phase, a Wigner supersolid state caused by dipolar repulsion in electron-hole bilayers, was described \cite{25}. The recent theoretical and experimental achievements in the studies of the superfluid dipolar exciton phases in CQWs were reviewed in Ref. \cite{1}, and various experimental studies of excitonic phases in CQWs were described in Ref. \cite{26}.

The formation of a superfluid with indirect excitons was recently proposed in Ref. \cite{27} using MoS\textsubscript{2} layers separated by a hexagonal boron nitride insulating barrier and surrounded by hexagonal boron nitride cladding layers and in Ref. \cite{28} for dipolar excitons in two parallel transition metal dichalcogenides layers. A perpendicular electric field modifies the band structure in a way that it becomes advantageous for optically excited electrons and holes to reside in the opposite MoS\textsubscript{2} monolayers to form indirect excitons. As an extension of these proposals, we consider excitons in a somewhat modified design, using a structured gate to create an additional periodic potential, to study the linear response of the excitonic superfluid to an electromagnetic wave at low and high concentrations. This provides a new controllable scale through the length of the periodicity.

Besides the question about how to create collective states in an exciton gas it is also important to characterize and analyze these states experimentally. Although the system is assumed to be translational invariant, there are characteristic spatial correlations of quantum fluctuations. Here we suggest to measure...
the linear response to an external electromagnetic field. This response depends on the wavevector \( \mathbf{q} \) of the external field, which provides information related to the spatial properties of the state. Using the static structure factor (SSF), the response is related to the spatial correlation function of the exciton density \[29\]. In this paper we will study the SSF inside the superfluid phase and how it changes when we get close to the phase boundaries in the dilute regime and in the high density regime (i.e., near the transition to an MI phase).

The paper is organized in the following way. In Sec. \[II\] starting from an interacting gas of electrons and holes, we derive an effective model for excitons formed by bound electron-hole states. Assuming Coulomb interaction, we neglect the possibility for a dissociation of electrons and holes. This model is treated in mean-field approximation and the Green’s function of quasiparticles are calculated in Subsect. \[II.A\]. In Sec. \[III.A\] we study the corresponding SSF at non-zero temperature and compare it with the result of zero temperature. The results are discussed for different regimes in Sec. \[IV\]. Conclusions follow in Sec. \[V\].

II. MODEL OF A ELECTRON-HOLE GAS IN AN EXTERNAL PERIODIC POTENTIAL

The Hamiltonian of a the system of electrons and holes, either in single layer or spatially separated in a double layer, can be written in momentum representation as

\[
H = \sum_{\mathbf{p}} \sum_{\sigma = e, h} (\epsilon_{\mathbf{p}, \sigma} - \mu_{\sigma}) c_{\mathbf{p}, \sigma}^{\dagger} c_{\mathbf{p}, \sigma} + \sum_{\mathbf{p}, \mathbf{p}', \mathbf{p}'', \mathbf{p}''} U_{\mathbf{p}, \mathbf{p}'} c_{\mathbf{p}', \mathbf{p}''}^{\dagger} c_{\mathbf{p}''} c_{\mathbf{p}, \mathbf{p}'} c_{\mathbf{p}, \mathbf{p}''},
\]

where \( c_{\mathbf{p}, \sigma}^{\dagger} \) (\( c_{\mathbf{p}, \sigma} \)) is the creation (annihilation) operator for electrons, and \( c_{\mathbf{p}, h}^{\dagger} \) (\( c_{\mathbf{p}, h} \)) are the corresponding operators for holes. While \( \mu_1 \) is the chemical potential of electrons, \( \mu_2 \) is the chemical potential of holes, assuming the concentrations of electrons and holes are equal in order to have a neutral electron-hole plasma. This is justified since the electrons and holes are created always pairwise by an external laser source. The electron and hole single-particle energy spectra \( \epsilon_{\mathbf{p}, \sigma} \) are defined in a tight-binding approximation, reflecting an external periodic field which is applied to the system. The electron-hole attraction due to Coulomb interaction is given in momentum space as \( U_{\mathbf{p}} \), which is finite for \( q \sim 0 \) as a result of screening. Its specific form is different whether we have direct or indirect excitons. In Eq. \[II\] the spins of electrons and holes are neglected, because we are not interested in magnetization effects.

The fermionic Hamiltonian could be treated within the BCS mean-field approximation to obtain the order parameter for Cooper pairs \[3\]. For many physical quantities, such as the superfluid concentration, this approximation is sufficient. Correlations of excitons, though, would also require to include quantum fluctuations generated by quasiparticles. There are several options for including quantum excitonic effects. A very direct way is to consider an effective Hamiltonian \( H_b \) which describes the dynamics of excitons on the lattice, based on tunneling of excitons between neighboring lattice sites. When we assume that the effect of the Coulomb interaction is strong, for instance, in case of a small distance between electrons in one and holes in another layer, the excitons will not dissociate into electrons and holes. Then we can consider the excitons as stable quantum particles, where the shortest distance of the model is the lattice spacing, because the excitons tunnel between the neighboring minima of the periodic potential. The fact that excitons are formed by fermions leads to a local repulsive interaction. Similar to the famous Hubbard model, the competition of nearest neighbor tunneling on the lattice and the on-site repulsion can lead to the rich physics of “strong correlations” with different quantum states, including superfluidity, Mott and topological states. This requires the tuning of the tunneling rate and the concentration of particles. Both parameters are tunable in our experimental proposal through the variation of an external electric field.

A. Effective exciton model

First, the idea is to derive from the fermionic Hamiltonian \[II\] an effective Hamiltonian for bound electron-hole pairs (excitons) whose creation operators in configuration space can be written as

\[
a_{\mathbf{r}}^{\dagger} = \int d^2 r' d^2 r'' K_{\mathbf{r} - \mathbf{r}', \mathbf{r} - \mathbf{r}''} c_{\mathbf{r}', h}^{\dagger} c_{\mathbf{r}'}^{\dagger} c_{\mathbf{r}, e} c_{\mathbf{r}', e} d^2 r' d^2 r'',
\]

(2)
where the kernel $K_{r-r',r-r''}$ decays exponentially on a characteristic length $\xi$ away from $r$. This length represents the effective size of the exciton. Now we assume that the lattice spacing is much larger than $\xi$, which implies that the exciton creation and annihilation operators are in a good approximation local:

$$a_r^\dagger = c_r^\dagger e_r^\dagger, \quad a_r = c_r e_r^\dagger. \tag{3}$$

These operators resemble hard-core bosons, since they satisfy the bosonic commutation relations with the additional condition $a_r^2 = 0$ due to the Pauli principle of the fermionic constituents.

Second, we assume that the excitons cannot dissociate into fermions. Therefore, the effective Hamiltonian is expressed by the operators $a_r$ and $a_r^\dagger$ only. As a first order approximation we can write

$$H_{eff} = \sum_{r,r'} (J_{r,r'} + \mu \delta_{r,r'}) a_r^\dagger a_{r'}, \tag{4}$$

where the summation is with respect to the minima of the periodic potential, using a tight-binding approximation. In Eq. (4) the hopping rate is

$$J_{r,r'} = \begin{cases} J, & \text{r, r’ nearest neighbors} \\ 0, & \text{otherwise} \end{cases} \tag{5}$$

describes the tunneling of excitons between neighboring potential minima, while $\mu$ is the chemical potential of excitons that controls their concentration. This Hamiltonian describes essentially the physics of the exciton gas in a periodic potential with on-site interaction. Its extension to other types of interaction, including long-range dipole-dipole interaction, is obvious but not important for the subsequent discussion.

Hamiltonian (4) can have a normal and a superfluid state for the exciton gas. In particular, the MI state with concentration $n_{tot} = 1$ is an eigenstate of $H_{eff}$. Considering that the system is at temperatures well below the Kosterlitz-Thouless transition temperature, one can use a mean-field approximation and follow the idea of the Bogoliubov approach. Then the superfluid phase is distinguished from the normal phase by a spatially uniform order parameter $\phi = |\phi| e^{i\alpha}$, which vanishes outside the superfluid phase. Then the exciton operators in the superfluid phase read

$$a_r = \phi + \varphi_r, \quad a_r^\dagger = \phi^* + \varphi_r^\dagger, \tag{6}$$

where $\varphi_r^\dagger$ is the creation operator for bosonic quasiparticles. If $N_0$ is the number of bosons in the superfluid phase and $N$ is the number of lattice sites, $n_0 = N_0/N$ is the concentration of superfluid excitons per unit cell of the lattice. $N_0$ is obtained from the order parameter as $N_0 = |\phi|^2$. A mean-field approximation for the Hamiltonian (4) gives at zero temperature [31, 32]

$$n_0 = \begin{cases} \left(1 - \mu^2/J^2\right)/4, & \text{if } -1 < \mu/J < 1 \\ 0, & \text{otherwise} \end{cases} \tag{7}$$

Moreover, the total excitonic concentration $n_{tot} = N_{tot}/N$ per unit cell of the lattice is obtained from the free energy per site

$$F = -\frac{1}{\beta N} \log \left(\text{Tr} e^{-\beta H_k}\right) \tag{8}$$

as

$$n_{tot} = \frac{\partial F}{\partial \mu} \sim \begin{cases} 0, & \text{if } \mu/J \leq -1 \\ (1 + \mu/J)/2, & \text{if } -1 < \mu/J < 1 \\ 1, & \text{if } \mu/J \geq 1 \end{cases} \tag{9}$$

Therefore, concentrations are measured in units of the lattice constant and appear in our calculation as dimensionless quantities.

In Fig. 2 the total and the superfluid concentration are plotted in the superfluid phase, shown in Fig. 1 as a function of the chemical potential. In the dilute regime, that corresponds to low total concentration, almost all excitons are in the superfluid phase, whereas a reduction of the superfluid concentration with increasing total concentration is caused by the formation of a kind of supersolid due to the interplay of the interaction and the underlying lattice structure.
FIG. 1: Excitonic phase diagram at $T = 0$ with three different phases, separated by two second-order transition lines (from Eq. (7), in arbitrary units). The lower phase is a MI phase with $n_{\text{tot}} = 0$, $n_0 = 0$, the upper phase is a MI phase with $n_{\text{tot}} = 1$, $n_0 = 0$ and the intermediate phase is a superfluid phase with $0 < n_{\text{tot}} < 1$, $n_0 > 0$. The concentrations along a vertical cut through the intermediate phase at a fixed hopping rate $J$ are plotted in Fig. 2.

FIG. 2: The total excitonic concentration $n_{\text{tot}}$ (dashed curve) and the condensate concentration $n_0$ (solid curve) in mean-field approximation (cf. Eqs. (7) and (9)) for $-1 \leq \mu/J \leq 1$, where the normalized chemical potential is $\mu/J$. Lattice effects prevent that all excitons participate in the superfluid as the concentration is increasing, indicating a crossover to a MI state.

The rather simple results in Eqs. (7) and (9) can be used to calculate other physical quantities of the excitonic gas. For instance, the effect of quantum fluctuations in momentum representation is described by the quasiparticle Green’s function of $\delta \phi_q = \hat{\phi}_q + \hat{\phi}_q^\dagger$:

\[
\langle \delta \phi_{q,\omega} \delta \phi_{-q,\omega} \rangle = \frac{(1 - \kappa_q^2)(1 + 1/\kappa_q)}{(1 - \kappa_q^2)[2n_0 - 1/2 + 1/(1 + \kappa_q)] - (\hbar \omega/J)^2},
\]

where $\kappa_q$ is the dispersion in the periodic potential, normalized with $J$, and $\omega$ is the frequency of the external electromagnetic field. This result is similar to the two-particle Green’s function obtained for the exciton gas in Ref. [33].
### III. STATIC STRUCTURE FACTOR

The response of a many-body quantum system to a weak external electromagnetic field of frequency $\omega$ and wavevector $\mathbf{q}$ is given by Fermi's Golden Rule, where the latter is characterized by the structure factor $S(\mathbf{q}, \omega)$ [28, 34]. This quantity is defined as the Fourier transform of the truncated density-density correlation function:

$$S(\mathbf{q}, \omega) = \frac{1}{2\pi n_{\text{tot}}} \int_{-k_p} \int \left[ \langle \hat{a}_k(t) \hat{a}^\dagger_{k-\mathbf{q}}(t) \hat{a}^\dagger_{\mathbf{p}-\mathbf{q}}(0) \rangle - \langle \hat{a}_k(t) \hat{a}^\dagger_{k-\mathbf{q}}(t) \rangle \langle \hat{a}_{\mathbf{p}}(0) \hat{a}^\dagger_{\mathbf{p}-\mathbf{q}}(0) \rangle \right] e^{i\omega t} dt d^2p d^2k,$$

where the wavevector $\mathbf{q}$ is measured in units of the inverse lattice constant $1/a$. Using the truncated correlation function (i.e., subtracting the product of concentrations by the second term) eliminates a Dirac delta function at $\mathbf{q} = 0$.

With the operators in Eq. (6), $\phi = \sqrt{N_0}$ and the quasiparticle Green's function [10] we obtain

$$S(\mathbf{q}, \omega) = \frac{n_0}{n_{\text{tot}}} \langle \delta \phi_{\mathbf{q}, \omega} \delta \phi_{-\mathbf{q}, \omega} \rangle .$$

Integration over all frequencies $\omega$ gives us the SSF as

$$S(\mathbf{q}) = \frac{1}{2\pi} \int S(\mathbf{q}, \omega) d\omega = \frac{n_0}{4n_{\text{tot}}} \frac{(1 - \kappa_q^2)(1 + 1/\kappa_q)}{\sqrt{(1 - \kappa_q^2)[2n_0 - 1/2 + 1/(1 + \kappa_q)]}}$$

with the lattice tight-binding dispersion $\kappa_q$. In the case of a square lattice with lattice constant $a$ we get $\kappa_q = (\cos aq_1 + \cos aq_2)/2$. Replacing $J(1 - \kappa_q)$ by the dispersion of a free Bose gas $\hbar^2 q^2/2m$ and assuming that $\hbar^2 q^2/2m \ll J$, we obtain from Eq. (13) the well-known result of Feynman for the low concentration regime $n_0/n_{\text{tot}} \sim 1$ [35]:

$$S(\mathbf{q}) \sim \frac{\hbar^2 q^2/2m}{\sqrt{(\hbar^2 q^2/2m)[4Jn_0 + \hbar^2 q^2/2m]}} .$$

#### A. Thermal fluctuations

The SSF at zero temperature is characterized by a vanishing behavior for a vanishing wavevector $\mathbf{q}$. The question is now whether or not this behavior is also visible in a realistic experiment where we have thermal fluctuations. We will demonstrate subsequently that this is not the case, since even very small thermal fluctuations alter the behavior of the SSF substantially at small wavevectors.

The calculation for including thermal fluctuations requires a summation with respect to Matsubara frequencies $\omega_l = 2\pi l/\beta \hbar$, where $l = 0, 1, 2, ...$ [35, 39], rather than a frequency integration. This summation can be expressed again by an integral in the complex plane [37], which gives us for the superfluid phase [29, 31, 32]

$$S(\mathbf{q}) \sim \frac{n_0}{n_{\text{tot}}} \frac{g_\mathbf{q}}{\epsilon_\mathbf{q}} \coth \frac{\beta J q^2}{2} \text{ with } \epsilon_\mathbf{q} = \sqrt{4n_0 g_\mathbf{q} + (1 - 4n_0) g_\mathbf{q}^2}$$

and with the bare dispersion $g_\mathbf{q} = 1 - (\cos aq_1 + \cos aq_2)/2$ for the square lattice. The SSF is very sensitive to thermal fluctuation at small $\mathbf{q}$, as illustrated in Fig. 4 for $n_0 = 0.0025$: It vanishes for $T = 0$ and $\mathbf{q} = 0$, whereas it increases strongly for $3J = 0.01$ if $\mathbf{q} \sim 0$. The reason for this behavior is the coth $x$ term, which diverges for $x \sim 0$. This factor is 1 for strictly zero temperature but diverges for any finite $\beta$ when $\mathbf{q} \sim 0$.

### IV. DISCUSSION

Let us distinguish three different regimes for the SSF: $\mu \sim -J$ (low concentration regime), $\mu = 0$ (maximum superfluid concentration) and $\mu \sim J$ (vanishing superfluid at high concentration). For the
behavior of the SSF it is crucial that the limit $T \to 0$ followed by the limit $q \to 0$ leads to a different result for the structure factor than the limit $q \to 0$ followed by the limit $T \to 0$. Therefore, we have to be careful with the regime $q \sim 0$ at low temperature, because the SSF is very sensitive to small changes of parameters. This can be seen in Figs. 3, 4 where either a small change in temperature or a small change in the superfluid concentration has a strong effect on the SSF.

i. Low concentration regime In the dilute regime with $\mu \sim -J$ we have $n_0/n_{\text{tot}} = 1$, such that we obtain from Eq. (15)

$$S(q) \sim \frac{g q}{\epsilon_q} \coth \frac{\beta J \epsilon_q}{2} \sim \coth \frac{\beta J \epsilon_q}{2} ,$$

(16)

which is in agreement with the well-known result for the weakly interacting Bose gas and with the SSF of the ideal (noninteracting) Bose gas $\frac{2}{\beta J g_q}$. For low concentration, when $\beta J \epsilon_q \ll 1$ one can obtain from Eq. (16)

$$S(q) \sim \frac{2}{\beta J g_q} .$$

(17)
Interaction between the excitons can have two effects: it can create a superfluid with concentration \( n_0 > 0 \) and, together with the periodic potential, it can destroy the superfluid and create a MI state. Thus, besides the weakly interacting regime with \( n_{\text{tot}} \sim n_0 \sim 0 \), there is an intermediate regime with \( n_{\text{tot}} \sim 0.5 \) and maximum superfluid concentration \( n_0 \sim 0.25 \), and a strongly interacting regime of a dense exciton gas with \( n_{\text{tot}} \sim 1 \) and \( n_0 \sim 0 \).

### ii. Maximum superfluid concentration

In this case we have \( \mu = 0 \), which implies according to Eqs. (7) and (9) \( n_0 = 1/4 \) and \( n_{\text{tot}} = 1/2 \) (half-filled lattice); i.e., \( n_0/n_{\text{tot}} = 1/2 \). Moreover, we get for the quasiparticle dispersion \( \epsilon_q = \sqrt{g_q} \) and, therefore,

\[
S(q) \sim \frac{1}{2} \frac{g_q}{\epsilon_q} \coth \frac{\beta J \epsilon_q}{2} \sim \frac{1}{2} \sqrt{g_q} \coth \frac{\beta J \sqrt{g_q}}{2} \sim \frac{1}{\beta J} \text{ for } \beta J \sqrt{g_q} \ll 1. \tag{18}
\]

### iii. High concentration regime

\( \mu \sim \epsilon_q \) implies for the concentrations \( n_0 \sim 0 \) and \( n_{\text{tot}} \sim 1 \); i.e., \( n_0/n_{\text{tot}} \sim 0 \). Thus, in the dense regime, i.e. close to the MI phase when \( n_{\text{tot}} \approx 1 \), the SSF vanishes with \( n_0 \) as

\[
S(q) \sim n_0 \frac{g_q}{\epsilon_q} \coth \frac{\beta J \epsilon_q}{2} \sim \frac{1}{2} \frac{1}{1 + g_q/4n_0 \beta J} \text{ for } \beta J \epsilon_q \ll 1. \tag{19}
\]

in contrast to Eq. (17) for the dilute regime.

The dependence of the SSF on \( g_q \) in the dilute regime is depicted in Fig. 3. At fixed temperature the SSF is plotted in Fig. 4 for different values of \( n_0 \). Both figures reflect the asymptotic behavior for small \( q \) obtained in Eqs. (17), (18) and (19). In the experiment with a dilute exciton gas we should always see a broad maximum at small \( q \) which decays according Eq. (17) like \( q^{-2} \). This maximum disappears at higher exciton concentrations, and the SSF is relatively flat with a very weak increase, as illustrated in Fig. 4.

We have not calculated the SSF in the MI phase because the latter is not accessible with the present experimental techniques. Such a calculation would require a different approach to obtain the corresponding quasiparticle Green’s function. But this is a straightforward task when we use the concept developed, for instance, in Ref. [31].

### V. CONCLUSIONS

We predict a method to control the state of an exciton system by introducing a spatially periodic potential through a profiled external gate or by a periodic superlattice structure. The control can be...
performed also by change of the chemical potential of the system, driven by laser pumping. The transition of superfluid (BEC) state to localized state takes place. This phase transition is controlled by the parameters of the external potential. The transition can be revealed by study of exciton flow induced by a gradient of the exciton concentration, originated from a photon pumping spot. Besides, the transition can be observed by elastic light scattering. The elastic light scattering cross section is proportional to the static structure factor. We demonstrated that the static structure factor drastically changes at the superfluid to localized states transition.

The SSF, which can be measured by non-resonant scattering of electromagnetic waves, is a useful quantity to characterize a superfluid state in an excitonic system. Since the latter was proposed some time ago [24] and observed in a recent experiment [38], a detailed analysis, for instance, based on X-ray Raman scattering (XRS) [39] could reveal more details of the nature of this state. In particular, there is a pronounced maximum of the SSF at small wavevectors in the case of a dilute exciton gas and an almost flat SSF at higher exciton concentrations. This high sensitivity can be employed for accurate measurements of the superfluid properties at small wavevector $q$. In particular, it would be possible to observe the reduction of the superfluid concentration and the crossover to the MI phase under an increasing total exciton concentration. In a proper experimental set-up the latter could be controlled by an external gate.

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