Numerical Study of the Vortex Phase Diagram Using the Bose Model in STLS approximation

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We study the phase diagram of the flux lines using the mapping to 2D bosons in the self-consistent-field approximation of Singwi, Tosi, Land, and Sjolander (STLS). The pair correlation function, static structure factor, interaction energy, and spectrum of the excited energies are calculated over a wide range of the parameters in this approximation. These quantities are used for studying the melting transition from the Abrikosov lattice into the entangled vortex liquid. The resulting $B-T$ phase diagram is in good agreement with the known estimates for the vortex lattice melting and the Monte Carlo simulations. We also discuss the effect of van der Waals interaction, induced by thermal fluctuations, together with the repulsion potential on the phase diagram.

I. INTRODUCTION

The phases of flux lines (FLs) in high temperature superconductors are the subject of many current experimental and theoretical investigations. In the classical (Abrikosov) picture of type-II superconductors, FLs penetrate a clean material for fields $H > H_{c1}$, to form a triangular solid lattice. This mean field phase diagram is modified by inclusion of the strong thermal fluctuations and play an important role in high-$T_c$ materials. The presence of various forms of disorder (such as point or columnar disorder) also affects on the mean field phase diagram. In this paper we typically focus on the phase diagram of the pure materials, however, there are many interesting experimental and theoretical works describing the effect of both thermal fluctuations and disorder on the phase diagram.

It is well known that the thermal fluctuations lead to melting of the vortex lattice and appearance of a vortex liquid. It has now become possible to observe the melting transition experimentally. The indirect observations based on the resistivity measurements, and recent experiments based on the measuring a jump in the magnetization or the latent heat show a first-order vortex lattice melting transition. On the other hand, vortex lattice melting has been studied theoretically using various approximations. Early works using the renormalization group or density functional theory have indicated a first-order transition. Elastic theory combined with the Lindemann criterion produce a melting line in good agreement with the experimental observations. There are also a large interest in numerical simulations for studying this problem. An interesting work in this direction is done by Nordborg and Blatter which present an extensive numerical study of the vortex matter using the mapping to 2D bosons and path-integral Monte Carlo simulations.

It was suggested by Nelson that the vortex system is equivalent to a system of interacting bosons in two dimensions (Bose model). This mapping predicts a melting transition into an entangled vortex liquid. Therefore, the problem of a vortex system maps to a system of $N$ bosons in two dimensions interacting through the potential $V(r) = g^2 K_0(r/\lambda)$, where $K_0$ is the modified Bessel function, $\lambda$ is the London penetration depth, and $g^2$ is a constant that scales the energy of interaction. In the language of the vortices, this potential comes from the interaction between vortices in the London theory, and $g$ is related to the elastic moduli of the vortex lattice. The Bose model differs from the real vortex system (see next section), however it still contains the main part of the interaction. Hence, it would be reasonable and interesting to use this model for describing the properties of the vortex phase diagram. More recently, the Bose model has been used in a numerical study of the vortex matter. Some physical quantities such as structure factor and superfluid density in different temperatures are given addressed, and the first order vortex lattice melting transition into an entangled vortex liquid is approved by numerical simulations. In the language of the boson system, this transition is related to the quantum phase transition from a Wigner crystal to a superfluid.

The Bose model idea also allows for using the many body techniques. In this work, we apply the self-consistent-field approximation of Singwi, Tosi, Land, and Sjolander (STLS), and calculate the static structure factor, pair correlation function, interaction energy and the spectrum of the excited energies for different magnetic field strengths and temperatures. The STLS approximation has originally been proposed for describing a degenerate electron gas and has been used successfully to study a variety of other systems too. In the STLS theory, the correlation effects are incorporated through a static local-field correction, which is obtained numerically in a self-consistent way. We find numerical results for the static structure factor $S(q)$ over a wide range of the parameters. From the calculation of $S(q)$, we present the results for the pair correlation function, the interaction energy and spectrum of the excited energies. Different behaviors of these quantities may be used for studying the phases of vortex lines.

It is well known that the oscillatory behavior in $g(r)$
is a signature of the solid phase. Therefore, the phase transition can be detected by looking at the behavior of the \( g(r) \) in a fixed temperature (magnetic field) but varying magnetic field (temperature). The solid-liquid transition can also be observed using the static structure factor. Disappearing of the peaks in the structure factor resembles the onset of the phase transition. Hence, using the behaviors of the pair correlation function and static structure factor, the phase diagram can be explained qualitatively, however, it is not possible to determine precisely the melting transition temperature.

One of the transition signatures is the appearance of a special \( q \) on which the spectrum of the excited energies vanishes. So we have numerically investigated the dispersion relation of the excited energies as a good quantity for the estimation of the \( B - T \) phase diagram and the melting temperature. Quantitatively our results for the excited energies are compatible with the expected results of the phase diagram \([1]\) and recent Monte Carlo simulations \([2]\).

On the other hand, the direction dependent interaction for real vortices has very interesting consequences and predicts a van der Waals interaction even for straight vortices \([2]\). It is shown \([2,23]\) that in the decoupled limit, \( \gamma \to 0 \) (where \( \gamma \) is the anisotropy parameter), the van der Waals attraction is proportional to \( 1/R^2 \). This attractive interaction with entropic repulsion has very important outcomes for the low-field phase diagram of the anisotropic superconductors \([2,23,24]\). Recently Volmer and Schwartz \([26]\) introduced a new variational approach to consider the effects of van der Waals attraction and repulsive interaction on the field phase diagram. We also consider the same model in the STLS approximation for studying the combined effects of the repulsive and attractive potentials on the solid and liquid phases of the pure anisotropic or layered superconductors.

The rest of this paper is organized as follows. In Sec. II, we shortly review the Bose model and discuss its applicability to the vortex system. The STLS approximation is briefly discussed in Sec. III. The numerical results for the repulsion interaction is presented and discussed in the Sec. IV. The results for the van der Waals interaction and its consequences in the phase diagram is given in Sec. V, and finally the conclusions appear in Sec. VI.

II. BOSE MODEL

In the Feynman path-integral picture \([27]\), the system of \( N \) interacting bosons in two dimensions is described by the action

\[
\frac{S}{\hbar} = \frac{1}{\hbar} \int_0^{h/T} d\tau \left\{ \sum_i \frac{M}{2} \left( \frac{d\vec{R}_i}{d\tau} \right)^2 + \sum_{i<j} g^2 K_0 \left( \frac{R_{ij}}{\lambda} \right) \right\},
\]

(1)

where \( \vec{R}_i(\tau) \) is a two dimensional vector representing the positions of the bosons, and \( T \) is the temperature of the system. In the Schrodinger picture the above action is equivalent to the two-dimensional Schrodinger equation,

\[
\left[ -\sum_i \nabla_i^2 + \sum_{i,j} V(R_{ij}) \right] \psi_0 = E_0 \psi_0,
\]

(2)

where the potential \( V(R_{ij}) \) is proportional to the modified Bessel function.

It was pointed out by Nelson \([4,7]\) that the above action can be also interpreted as the London free energy for a system of vortex lines. The London free energy for a system of interacting vortices for a sample of length \( L_z \) is given by,

\[
\mathcal{F} = \frac{1}{T} \int_0^{L_z} dz \left\{ \sum_1 \varepsilon_l \left( \frac{d\vec{R}}{dz} \right)^2 \right\} + \sum_{i<j} 2\varepsilon_0 K_0 \left( \frac{R_{ij}}{\lambda} \right),
\]

(3)

where \( \varepsilon_l \approx \gamma^2 \varepsilon_0 a_0/(2\sqrt{\pi} \xi) \), \( \varepsilon_0 = (\Phi_0/4\pi \lambda)^2 \), \( \Phi_0 \) is the quantum flux, \( \xi \) is coherence length, and \( a_0 \) is the lattice spacing. Comparing this functional free energy, which is referred as Bose model for the vortex system, with the action \([1]\) shows the relationship between the parameters of the 2D bosons and vortices.

The modified Bessel function \( K_0(R/\lambda) \) describes a screened logarithmic interaction, \( K_0(x) \sim -ln x \) for \( x \to 0 \), and \( K_0(x) \sim x^{-1/2}e^{-x} \) for \( x \to \infty \). Thus, the London penetration depth defines the interaction range. Note that according to the two-fluid model \([18]\), the penetration depth diverges at zero-field transition temperature \( T_c \), and therefore the interaction range becomes considerably longer upon approaching \( T_c \).

As it is discussed in details in the Ref. \([20]\), in spite of the fact that the Bose model differs from the real vortex system in the choice of boundary conditions, the linearization leading to the elastic term, and the retarded interaction, contain the main parts of the interaction between vortices and one expects that the results be in a rough quantitative agreement with those of real systems.

III. STLS APPROXIMATION

In this section we shortly review the principal equations of the STLS approximation \([23]\). These equations show the relation between the response function, static structure factor, and the local field correction.

In the STLS approximation, the response function can be expressed as \([23]\),

\[
\chi(q,\omega) = \frac{\chi_0(q,\omega)}{1 - \psi(q)\chi_0(q,\omega)}.
\]

(4)

In this equation \( \chi_0 \) is the response function of the free Bose gas and \( \psi \) is the effective potential given by \( \psi(q) = \frac{1}{\hbar^2} \int_0^{h/T} d\tau \left\{ \sum_i M \left( \frac{d\vec{R}_i}{d\tau} \right)^2 + \sum_{i<j} g^2 K_0 \left( \frac{R_{ij}}{\lambda} \right) \right\} \) is the energy of the system. In the STLS approximation, the response function can be expressed as \([23]\),

\[
\chi(q,\omega) = \frac{\chi_0(q,\omega)}{1 - \psi(q)\chi_0(q,\omega)}.
\]

(4)
The STLS local field correction is of the bare potential, and poles of Eqn. (4), leading to
ture factor.

For a noninteracting two dimension Bose gas the free re-

where \( n \) is the density, and \( S(q) \) is the static structure factor and is related to response function as (\( \hbar = 1 \)),

\[
S(q) = \frac{1}{(n\pi)} \int_{0}^{\infty} d\omega \text{Im}(\chi(q, \omega)).
\]  

For a noninteracting two dimension Bose gas the free re-

\[
\chi_0(q, \omega) = \frac{2n\epsilon(q)}{[(\omega + i\eta)^2 - \epsilon(q)^2]}.
\]  

where \( \epsilon(q) = q^2/(2m) \) is the free particle energy, and \( \eta \) is a positive infinitesimal quantity.

Using the Eqn. (6), one can calculate the integral

Eqs. (5) and (8) should be solved numerically for

\[
E_{\text{int}} = \frac{1}{4\pi} \int_{0}^{1} d\lambda \int_{\lambda}^{1} v_\lambda(q)(S_\lambda(q) - 1)q dq.
\]  

where \( v_\lambda(q) = \lambda v(q) \) and \( S_\lambda(q) \) is its related static structure factor.

One can also compute the excited energy using the poles of Eqn. (4), leading to

\[
\omega(q) = \sqrt{\epsilon^2(q) + 2n\epsilon(q)v(q)(1 - G(q))}.
\]  

In the next section, we present numerical results for various quantities of interest.

**IV. NUMERICAL RESULTS**

In this section we present the results of the numerical calculations for the interesting physical quantities. We numerically solve the set of Eqs. (5) and (8) with the repulsion potential defined in Eqn. (3), and find the static structure factor. The calculations are done for different values of the two parameters \( m \) and \( r_s \). For the boson system \( m \) can be considered as the mass of particles (in the unit of \( \hbar = 1 \)), and for vortex lines \( m \) is related to the temperature as \( m = \epsilon_0\lambda^2/T^2 \).

Substituting the numerical values for parameters as \( \epsilon_0 = 50K/A \), \( \gamma = 100 \), \( \lambda = 1000A \), the equivalent temperature will be fixed as \( T \approx 500/\sqrt{m}(K) \). On the other hand, \( r_s \) is the inverse of density corresponding to the particle density for boson system, or the density of FLs in the vortex matter. The mentioned relationship is expressed as \( B = \phi_0/\pi r_s^2 \lambda^2 \), or \( B \approx 0.06/r_s^2 \) (Tesla).

One of our numerical results which was developed by iterating the Eqs. (5) and (8) is the behavior of the static structure factor which is shown in Fig. 1 for a fixed \( r_s = 0.6 \) \((B \approx 0.17(Tesla))\) and different \( m \)'s (temperatures).

![Fig. 1: The static structure factor in terms of \( q \), for \( r_s = 0.6 \) and different \( m \)'s.](image)

Fig. 1 manifests the very expected behavior of the static structure factor, that is the peak of the \( S(q) \) is decreased by increasing \( T \) (decreasing \( m \)). Disappearing of the peak in the \( S(q) \) by increasing the temperature shows that the system undergoes a phase transition from the solid phase to the liquid phase.

We can also see the melting transition by fixing the temperature and increasing the magnetic field. Choosing \( m = 100 \) \((T = 50K)\), we have found the \( S(q) \) for different values of \( r_s \), see Fig. 2.
The amplitude of the peaks becomes smaller with decreasing the $r_s$, while it disappears for high magnetic fields. So we will have the same scenario for describing the phase transition.

The melting transition of the vortex lattice can also be discussed by studying the behavior of the pair correlation function. It is seen that the results of $S(q)$ can be used for calculating the $g(r)$ defined in the Eqn. (H). The results of $g(r)$ for $r_s = 0.4$ ($B \approx 0.38$(Tesla)) and different masses (temperatures) are plotted in Fig. 3.

We observe that the numerical results show that the interaction energy increases by decreasing the strength of magnetic field.

The results of the pair correlation function and static structure factor are in good qualitative agreement with the expected results of the phase diagram of the vortex system. However, for obtaining some quantitative description, we use the spectrum of the excited energy of the system. We have plotted the $\omega(q)$ in terms of $q$, see Fig. 4. Fixing the magnetic field but for varying temperatures, the following graph resembles that $\omega(q)$ tends to a zero value for a finite $q$. The appearance of minimum in $\omega(q)$ is in correspondence with the fact that $G(q)$ becomes greater than one for some ranges of $m$.

The system is going to have a transition from the solid phase to the liquid phase by increasing the temperature.

We have also determined the interaction energy of the system using the Eqn. (I). The results are shown in the Table 1.

| $r_s$ | $B$ | $E_{int}$ |
|-------|-----|----------|
| 0.1   | 6   | −2.15    |
| 0.2   | 1.5 | −1.78    |
| 0.4   | 0.38| −1.36    |
| 0.6   | 0.17| −1.09    |
| 0.8   | 0.09| −0.89    |
| 1     | 0.06| −0.74    |

Table 1: The interaction energy, in STLS approximation for $m = 50$ and different densities (The unit of magnetic fields is Tesla).

Fig. 2: The static structure factor for $m = 100$ and with different values of $r_s$.

Fig. 3 shows that the pair correlation function has oscillatory behavior for low temperatures, however, its amplitude becomes shorter by increasing the temperature, and disappears for very high temperatures. The oscillatory behavior is a signature of the solid phase, therefore,
However, we have realized by our numerical experience that when we are close to the transition point the $q$ value of the minimum $\omega(q)$ and the local field correction $G(q)$ are not highly sensitive to the variations of $m$. Therefore, at least for determining the transition temperature we have ignored their dependence to $m$ in the Eqn. (11). So we fixed the magnetic field and found the temperature that $\omega(q)$ becomes zero. The resulting $B-T$ phase diagram is plotted in the Fig. 5.

Fig. 5: The $B-T$ phase diagram of the flux lines. The solid line is the predicted result in Ref. [28] produced by Lin- demann criterion. Triangular points are the results of our numerical calculations.

Proceeding to fit our data with the known result $B = 4c_L^2 \phi_0 \varepsilon_0 \varepsilon_1/(\sqrt{3}T^2)$ [28,20], we found that the best fits can be achieved by fixing $c_L \approx 0.15$ and it is observed that the results are supporting the reports of Monte Carlo simulations [24].

V. VAN DER WAALS INTERACTION

Taking into account the direction dependent interaction for real vortices give rise to interesting results and predicts a van der Waals (vdW) interaction even for straight vortices [24]. Therefore, it would be interesting to consider the superposition of the short range attractive and the long range repulsive interactions and study its consequence for the low-field phase diagram of the anisotropic superconductors. It is shown [24,25] that in the decoupled limit, $\varepsilon \to 0$, the interaction potential is given by

$$V(R) = v_0 \left( K_0(R/\lambda) - a_{vdw} \phi(R/\lambda) \frac{\lambda^4}{R^4} \right), \quad (12)$$

where, $v_0 = 2\varepsilon_0/T$ measures the amplitude of the direct interaction between flux lines, and $a_{vdw}$ determines the strength of the thermal vdW attraction. The function $\phi(x)$ smoothly cuts off the power law part for $R < \lambda$ and is defined as,

$$\phi(x) = \begin{cases} 
0, & x \leq x_1 \\
\frac{1}{4} \left[ 1 + \sin \left( \frac{\pi (x_1 + x_2) / 2}{x_2 - x_1} \right) \right]^2, & x_1 < x < x_2 \\
1, & x \geq x_2 
\end{cases}$$

(13)

with $x_1 = 1$ and $x_2 = 5$. The choice of the cutoff function and the values of $x_1$ and $x_2$ is to some extent arbitrary [24,25]. The amplitude of the vdW attraction is given by $a_{vdw} \approx T/(2 \varepsilon_0 d \ln^2(\pi \lambda/d))$, where $d$ is the layer spacing. Using the BSCCO numerical values for the parameters, one finds that $a_{vdw} \approx 2 \times 10^{-5}T/K$ which is $2 \times 10^{-3}$ for the temperature $T = 100K$ close to critical temperature $T_c$ [25].

The potential defined in Eqn. (12) is applied for calculating the static structure factor in the STLS approximation. The results are plotted in the Fig. 6, where $A_{vw} = a_{vdw}v_0$.

Fig. 6: The static structure factor for fixed magnetic field $r_s = 0.2$ with different temperatures and strengths of the vdW attraction.

The results show that the importance of the vdW interaction with high magnetic field is valid only for the temperature close to the transition. One should note that the vdW interaction has very important consequences for low magnetic fields and temperatures. However, in our approach it is not possible to consider this case, and one has to use some other approximations or Monte Carlo simulations for seeing these effects.
VI. CONCLUSIONS

In this paper we studied the Bose model in STLS approximation. We found the static structure factor, pair correlation function, interaction energy and spectrum of the excited energies for different values of the mass (temperature) and the density (magnetic field). We discussed that how the results may be applied for the vortex matter phase diagram. If one fixes the magnetic field (temperature) and calculate \( S(q) \) for different temperatures (magnetic field), the gradual disappearance of the peaks in \( S(q) \) manifests the existence of the phase transition. One can also use the pair correlation function for describing the melting transition. We showed that the changing behavior of \( g(r) \) from oscillatory to a rather smooth one can be explored within our numerical scheme so that the hallmark of the transition from solid phase to the liquid phase can be observed. The results were in good qualitative agreement with the phase diagram of the FLs. For estimation of the \( B-T \) phase diagram quantitatively, we invoke to the behavior of the excited energy spectrum, from which the resulting phase diagram supports the expected results of the high temperature superconductors and Monte Carlo simulation quite well.

We also added the van der Waals attractive potential and studied the effect of both repulsive and attractive potentials in the phase diagram. The results indicate that the vdW interaction for high magnetic field is only important for the temperatures close to the melting temperature. We emphasis that our approach doesn’t work for the low magnetic fields and hence, it would be interesting to use some other methods and determine the effects of both repulsive and attractive potentials in the low magnetic fields and temperatures.

To our knowledge this is the first time that the STLS approximation is applied for studying the vortex system, and our work show that STLS approximation is applicable for studying other aspects of the vortex systems and it might help to reveal some unknown properties in further investigations.

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[1] G. Blatter et. al., Rev. Mod. Phys. 66, 1125 (1994).
[2] E. H. Brandt, Rep. Prog. Phys. 58, 1465 (1995).
[3] A. I. Larkin and Y. N. Ovchinnikov, J. Low Temp. Phys. 34, 409 (1979).
[4] D. R. Nelson, Phys. Rev. Lett. 60, 1973 (1988); D. R. Nelson and H. S. Seung, Phys. Rev. B 39, 9153 (1989).
[5] M. P. A. Fisher, Phys. Rev. Lett. 62, 1415 (1989); D. S. Fisher, M. P. A. Fisher and D. A. Huse, Phys. Rev. B 43, 130 (1991).
[6] M. Kohandel and M. Kardar, Phys. Rev. B 59, 9637 (1999).
[7] D. R. Nelson and V. M. Vinokur, Phys. Rev. Lett. 68, 2398 (1992); Phys. Rev. B 48, 13060 (1993).
[8] U. C. Tauber and D. R. Nelson, cond-mat/95050024, preprint (1995).
[9] D. Ertas and M. Kardar, Phys. Rev. Lett. 69, 929 (1992); ibid. 73, 1703 (1994); Phys. Rev. B 53, 3520 (1996).
[10] M. Kohandel and M. Kardar, preprint (1999).
[11] H. Safar et. al., Phys. Rev. Lett. 69, 824 (1992).
[12] M. Charalampos, J. Chaussy and P. Lejay, Phys. Rev. B 45, 5091 (1992).
[13] E. Zeldov et. al., Nature375, 373 (1995).
[14] U. Welp et. al., Phys. Rev. Lett. 76, 4809 (1996).
[15] A. Schilling et. al., Nature 382, 791 (1996).
[16] M. Roulin, A. Junod and E. Walker, Science 273, 1210 (1996).
[17] E. Brezin, D. R. Nelson and A. Thiaville, Phys. Rev. B 31, 7124 (1985).
[18] S. Sengupta et. al., Phys. Rev. Lett. 67, 3444 (1991).
[19] A. Houghton, R. A. Pelcovits and A. Subdo, Phys. Rev. B 40, 6763 (1989); G. Blatter, V. B. Geshkenbein, A. I. Larkin, H. Nordborg, Phys. Rev. B 54, 72 (1996).
[20] H. Nordborg and G. Blatter, cond-mat/9612023, preprint (1997); cond-mat/9612023, preprint (1998).
[21] K. S. Singwi, M. P. Tosi, R. H. Land and A. Sjoland, Phys. Rev. 176, 589 (1968).
[22] K. S. Singwi and M. P. Tosi, Solid State Phys. 36, 177 (1981).
[23] R. K. Moudgil, P. K. Ahluwalia, K. Tankehwkar and K. N. Pathak, Phys. Rev. B 55, 544 (1997).
[24] G. Blatter and V. B. Geshkenbein, Phys. Rev. Lett. 77, 4958 (1996).
[25] A. Volmer, S. Mukherji and T. Nathermann, cond-mat/9808098, preprint (1998).
[26] A. Volmer and M. Schwartz, cond-mat/9806298, preprint (1998).
[27] R. P. Feynman, Statistical Mechanics, Addison-Wesely, Redwood City (1972).
[28] G. Blatter et. al., Phys. Rev. B 54, 72 (1996).