Ground-state energy of the adsorbed Bose liquid*

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The ground state of the quasi-two-dimensional Bose liquid in a periodic one-body potential is examined. The energy shift and density variation due to the periodic potential are calculated with a procedure which combines the paired-phonon analysis and canonical transformations. The results of this calculation are compared to the recent calculation of these effects which employed a correlated wave function and a cumulant expansion. The results are the same to lowest order. The advantages and disadvantages of each technique are explored.

I. INTRODUCTION

A recent paper[1] (hereafter referred to as NC) on the ground-state properties of the two-dimensional Bose liquid examined the effects of a one-body periodic potential on the adsorbed liquid. These effects were investigated with a variational technique which used a correlated wave function and a cumulant expansion of various matrix elements.[2] The correlated wave function contained both one- and two-body terms. A Fourier expansion was used for both the periodic potential and the one-body term in the wave function. The "smallness" of these Fourier coefficients justified the truncation of the expansion at a low order.

The wave function used in NC was separable in the coordinate normal to the surface plane. The problem was thereby transformed into a two-dimensional calculation with, of course, both the new one- and two-body interactions involving an average of the original interactions over the motion in the direction of the surface normal. Assuming that this projection into two dimensions has been carried out in accordance with the procedure in NC, the rest of this paper shall consider only the two-dimensional aspects of the problem. The two-dimensional wave function is[1]

$$\psi_{2D}=\prod_{i=1}^{N} e^{w(\vec{r}_i)/2}\psi_0(\vec{r}_1,\ldots,\vec{r}_N). \tag{1}$$

The ψ_0 term describes a class of correlations found in the uniform Bose liquid while the prefactor describes the periodic variation in ψ_{2D} generated by the one-body potential.

The work reported here is a reexamination of the physics of this problem using a calculational approach which differs from that used in NC. It is shown that the lowest-order term generated by the cumulant expansion can be generated with a much simpler technique, this technique being based upon the paired-phonon analysis of the Bose liquid.[3] Using the formalism of Ref. 3 (hereafter referred to as CF) coupled with the use of canonical transformations, these lowest-order terms are generated in a way which makes the physics of the calculation more transparent then the direct use of the cumulant expansion. Furthermore, this second approach provides an alternate path to calculation of the higher-order terms.

II. MODEL HAMILTONIAN

The calculation begins with the Hamiltonian of a Bose liquid in two dimensions written in the paired-phonon space. Using the Boson quasiparticle creation and destruction operators $\{\hat{a}_{\vec{p}}^{\dagger}, \hat{a}_{\vec{p}}\}$ defined by the two-dimensional version of Eq. (26) in CF, the Hamiltonian for the system without the external field is

$$H=\sum_{\vec{p}}(e_p+\omega_p)\hat{a}_{\vec{p}}^{\dagger}\hat{a}_{\vec{p}}+\frac{1}{2}\sum_{\vec{p}}\omega_p(\hat{a}_{\vec{p}}^{\dagger}\hat{a}_{-\vec{p}}^{\dagger}+\hat{a}_{\vec{p}}\hat{a}_{-\vec{p}}), \tag{2}$$

where the sum over $\vec{p}$ extends over all $\vec{p}$ in the plane. The quantities e_p and ω_p are given by

$$e_p=\hbar^2p^2/2mS_0(p), \tag{3a}$$

$$\omega_p=S_0'(p)/S_0(p)+(\hbar^2p^2/4m)[1-1/S_0(p)], \tag{3b}$$

where $S_0(p)$ is the structure factor calculated for the original Jastrow wave function and $S_0'(p)$ is the derivative of the generalized structure factor as defined in Sec. III of CF.

The inclusion of an external crystalline field means the addition of a term $\hat{H}_1$ to $\hat{H}_0$, where

$$\hat{H}_1=\sum_G U_{\vec{G}}\hat{\rho}_G=\sum_G U_{\vec{G}}[NS_0(G)]^{1/2}(\hat{a}_{\vec{G}}^{\dagger}+\hat{a}_{-\vec{G}}), \tag{4}$$

where the $U_{\vec{G}}$ are the Fourier coefficients of the external field, $\hat{\rho}_{\vec{G}}$ is the density fluctuation operator, and the $\{\vec{G}\}$ are the reciprocal-lattice vectors for the external field. In the second form for $\hat{H}_1$, the $\rho_{\vec{G}}$ have been rewritten in terms of the quasi-

particle operators. The quantity N is the total number of Bose particles in the system. The $\hat{H}_1$ term causes $\langle \hat{a}_{\vec{G}} \rangle$ in the exact ground state to be nonzero, that is there exists a Bose condensate in all states formed by $\hat{a}^\dagger_{\vec{G}}$ acting on the vacuum state. A simple technique to deal with such situations is the displacement transformation defined by[4]

$$\hat{a}^\dagger_{\vec{G}} = (N)^{1/2}\zeta^*_{\vec{G}} + \hat{\alpha}^\dagger_{\vec{G}}, \tag{5a}$$

$$\hat{a}^\dagger_{\vec{p}} = \hat{\alpha}^\dagger_{\vec{p}} \quad \text{for } \vec{p} \neq \vec{G}. \tag{5b}$$

Since $\zeta_{\vec{G}}$ is a c number, the transformation is unitary, thus conserving the Bose commutation relations. The transformed Hamiltonian is then

$$\begin{aligned}\hat{H} = \hat{H}_0 + \hat{H}_1 = {} & \sum_p (e_p + \omega_p)\hat{\alpha}^\dagger_{\vec{p}}\hat{\alpha}_{\vec{p}} + \frac{1}{2}\sum_p \omega_{\vec{p}}(\hat{\alpha}^\dagger_{\vec{p}}\hat{\alpha}^\dagger_{-\vec{p}} + \hat{\alpha}_{\vec{p}}\hat{\alpha}_{-\vec{p}}) + \sum_G U_{\vec{G}}[NS_0(G)]^{+1/2}(\hat{\alpha}^\dagger_{\vec{G}} + \hat{\alpha}_{-\vec{G}}) \\ & + \sum_G (e_G + \omega_G)\zeta^*_{\vec{G}}\zeta_{\vec{G}} + \frac{1}{2}\sum_G \omega_G(\zeta^*_{\vec{G}}\zeta^*_{-G} + \zeta_{\vec{G}}\zeta_{-\vec{G}}) + \sum_G (e_G + \omega_G)(\zeta^*_{\vec{G}}\hat{\alpha}_{\vec{G}} + \zeta_G\hat{\alpha}^\dagger_G) \\ & + \sum_G U_G[NS_0(G)]^{1/2}(\zeta^*_{\vec{G}} + \zeta_{-\vec{G}}) + \frac{1}{2}\sum_G \omega_G(\zeta^*_{\vec{G}}\hat{\alpha}^\dagger_{-\vec{G}} + \zeta^*_{-\vec{G}}\hat{\alpha}^\dagger_{\vec{G}} + \zeta_{\vec{G}}\hat{\alpha}_{-\vec{G}} + \zeta_{-\vec{G}}\hat{\alpha}_{\vec{G}}),\end{aligned} \tag{6}$$

where the sum over $\vec{p}$ is again over all $\vec{p}$. The value of $\zeta_{\vec{G}}$ can be found by setting $\langle \hat{\alpha}_{\vec{G}} \rangle = 0$. Because of the simple nature of $\hat{H}_0$, this condition also eliminates all linear terms in the transformed Hamiltonian. Requiring that $\langle \hat{\alpha}_G \rangle = 0$ for all time means $\langle [\alpha_G, \hat{H}] \rangle = 0$ where the commutator is the equal time commutator. Using this equation together with Eqs. (4) and (5) produces the equation for ζ_G:

$$(e_G + \omega_G)\zeta_{\vec{G}} + \omega_G\zeta^*_{-\vec{G}} = -U_{\vec{G}}[S_0(G)]^{1/2}. \tag{7}$$

Using the complex conjugate of Eq. (7) together with the real, symmetric nature of e_p and ω_p, $\zeta_{\vec{G}}$ is found to be given by

$$\zeta_{\vec{G}} = \zeta^*_{-\vec{G}} = -U_{\vec{G}}[S_0(G)]^{1/2}/(e_G + 2\omega_G). \tag{8}$$

Writing $\hat{\rho}_{\vec{G}}$ in terms of $\hat{\alpha}_{\vec{G}}$ and $\hat{\alpha}^\dagger_{\vec{G}}$

$$\begin{aligned}\langle \hat{\rho}_{\vec{G}} \rangle &= (N)^{1/2}[S_0(G)]^{1/2}[(N)^{1/2}\zeta^*_{\vec{G}} + (N)^{1/2}\zeta_{-\vec{G}}] \\ &= -N\frac{2U_{\vec{G}}S_0(G)}{e_G + 2\omega_G}.\end{aligned} \tag{9}$$

This equation is equivalent to Eqs. (34) and (36) in NC.

Using Eq. (8), one finds that all the linear terms disappear in Eq. (6). The remaining terms in Eq. (6) can be put into diagonal form[3] via a Bogoliubov transformation

$$\hat{\beta}^\dagger_{\vec{p}} = (\hat{\alpha}^\dagger_{\vec{p}} - D_p\hat{\alpha}_{-\vec{p}})/(1 - D_p^2)^{1/2}, \tag{10a}$$

$$\hat{\beta}_{\vec{p}} = (\hat{\alpha}_{\vec{p}} - D_p\hat{\alpha}^\dagger_{-\vec{p}})/(1 - D_p^2)^{1/2}. \tag{10b}$$

The function D_p can also be determined via the condition $\langle \hat{\beta}^\dagger_{\vec{p}}\hat{\beta}^\dagger_{-\vec{p}} \rangle = 0$. This condition diagonalizes the Hamiltonian because of the simple bilinear form of $\hat{H}_0$. The constant terms in Eq. (6) are not affected by the Bogoliubov transformation, nor do they affect the value of D_p. In this sense, the crystalline field does not *directly* affect the optimization of the Jastrow wave function. Nevertheless, there is a subtle feedback effect since the δE produced by these constant terms is given by

$$\delta E = -N\sum_{G\neq 0}\frac{U^2_{\vec{G}}S_0(G)}{e_G + 2\omega_G}, \tag{11}$$

and this term does depend upon the original Jastrow wave function. Equation (11), which is a result of inserting Eq. (8) into Eq. (6) is precisely Eq. (38) in NC. Furthermore, the determination of D_p via $\langle \hat{\beta}^\dagger_{\vec{p}}\hat{\beta}^\dagger_{-\vec{p}} \rangle = 0$ reproduces Eq. (29) in CF, namely

$$D_p = -\omega_p/[e_p + \omega_p + (e_p^2 + 2e_p\omega_p)^{1/2}]. \tag{12}$$

To go beyond the analysis outlined above, it is necessary to introduce quasiparticle interactions into $\hat{H}_0$.[5] It would then be possible to recalculate $\zeta_{\vec{G}}$ and D_p using $\langle \hat{\alpha}_{\vec{G}} \rangle = 0$ and $\langle \hat{\beta}^\dagger_{\vec{p}}\hat{\beta}^\dagger_{-\vec{p}} \rangle = 0$. These quasiparticle interactions must be included in order to generate the kind of terms generated by higher-order cumulants.

III. WEAK-PAIR-INTERACTION LIMIT

Equation (11) does not reduce to the exact single-particle result in the limit that the pair interaction goes to zero [$S_0(Q) = 1$]. The $S_0(Q) = 1$ limit of Eq. (11) is the single-particle result only to second-order in perturbation theory. However, if the displacement transformation is used directly on the exact single-particle Hamiltonian:

$$H = \sum_{\vec{p}}(\epsilon - \mu)\hat{b}^\dagger_{\vec{p}}\hat{b}_{\vec{p}} + \sum_{\vec{p},\vec{G}} U_{\vec{G}}\hat{b}^\dagger_{\vec{p}+\vec{G}}\hat{b}_{\vec{p}} \tag{13}$$

(where ϵ_p is the free particle kinetic energy and μ is the chemical potential), and the condition $\langle \hat{\alpha}_{\vec{p}} \rangle = 0$ is used to determine $\zeta_{\vec{G}}$, one finds

$$\epsilon_G\zeta_{\vec{G}} + \sum_{G_1} U_{\vec{G}-\vec{G}_1}\zeta_{\vec{G}_1} = \mu\zeta_{\vec{G}}, \tag{14}$$

which is the exact free-particle result.[6] Because

the $\hat{b}_{\vec{p}}^{\dagger}$ and $\hat{b}_{\vec{p}}$ are *particle* creation and destruction operators, there is a normalization constraint on the $\zeta_{\vec{G}}$, namely $\sum_G \zeta_{\vec{G}}^{*}\zeta_{\vec{G}} = 1$. The lowest value of μ gives the $T = 0$ chemical potential.

If we set $\delta E = \mu$ ($\mu = 0$ for $U_{\vec{G}} = 0$) then second-order perturbation theory gives

$$\delta E = -\sum_{\vec{G}} \frac{U_{\vec{G}}^2}{\epsilon_G}, \tag{15}$$

which is the $S_0(Q) = 1$ limit of Eq. (11). Thus the transformation to the paired-phonon space (with its concomitant replacement of the density fluctuation operator by a pair of Bose operators) produces an approximate treatment of the effects of the single-particle potential. The paired-phonon analysis requires that almost all Bose particles be in the zero-momentum state *when* the pair interaction is turned off. This can be seen from the equation which gives $\hat{\rho}_{\vec{k}}$ in terms of the Bose operators. However, when the $U_{\vec{G}}$ are "large," the exact ground state requires a significant mixing of the zero-momentum state with the plane-wave states associated with $\{G\}$. If the $U_{\vec{G}}$ are "small," then most particles will be in the zero-momentum state, the $\hat{\rho}_{\vec{k}}$ can be replaced by a sum of two Bose operators, and simultaneously the second-order perturbation correction will be sufficient.

The exact excited states of (13) are generated by the transformation

$$\hat{\beta}_{\vec{p}}^{\dagger\nu} = \sum_G \zeta_{\vec{G}}^{\nu *}(\vec{p})\hat{\alpha}_{\vec{p}+\vec{G}}^{\dagger}, \tag{16}$$

with $\vec{p}$ now restricted to the first Brillouin zone. It is straightforward to demonstrate that the $\zeta_{\vec{G}}^{\nu}$ which diagonalize $\hat{H}$ are given by

$$(\epsilon_{\vec{p}+\vec{G}} - \mu)\zeta_{\vec{G}}^{\nu}(\vec{p}) + \sum_{G_1} U_{\vec{G}-\vec{G}_1}\zeta_{\vec{G}_1}^{\nu}(\vec{p}) = \omega_p^{\nu}\zeta_{\vec{G}}^{\nu}, \tag{17}$$

with $\hat{H}$ given by

$$H = \sum_{p,\nu} \omega_p^{\nu}\hat{\beta}_{\vec{p}}^{\dagger\nu}\hat{\beta}_{\vec{p}}^{\nu}. \tag{18}$$

Extensions of this approach to the case with interactions between adatoms means the inclusion of the usual two-body terms into $\hat{H}$. The treatment of these terms then means using the transformation in Eq. (16) (essentially a transformation to a Bloch bases set) along with the displacement and Bogoliubov transformations used in the treatment of the Bose liquid. This approach would be useful in those cases where the adatom-substrate interactions dominate over the adatom-adatom interactions. However, in those cases (like ^{4}He on bare graphite) where the adatom-adatom interactions dominate over the adatom-substrate interactions, the model Hamiltonian of Eq. (6) is a better starting point.

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