Charge compressibility and quantum magnetic phase transition in MoS$_2$

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We investigate the ground-state properties of a monolayer MoS$_2$ incorporating the Coulomb interaction together with a short-range inter-valley interaction among charge particles between two valleys within the Hartree-Fock approximation. We consider four variables as independent parameters, namely homogenous charge (electron or hole) density, averaged dielectric constant, spin degree of freedom and finally Hubbard repulsion coefficient which mostly originates from 4$d$ orbits of Mo atoms. We find the electronic charge compressibility within the mean-field approximation and show that a non-monotonic behavior of the compressibility as a function of carrier density which is rather different from those of the two-dimensional electron gas. We also explore a paramagnetic-to-ferromagnetic quantum phase transition for the wide range of the electron density in the parameter space.

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I. INTRODUCTION

Developments in the techniques of molecular beam epitaxy and chemical vapor deposition have allowed the fabrication of semiconductor structures in which the carriers can form a low-density fluid moving in low dimensionality [1]. Many of the electron-electron interaction effects become increasingly important as carrier density or dimensionality is reduced and the homogeneous electron gas where an assembly of fermions interacting by the Coulomb interaction and moving in a uniform neutralizing background provides a primitive model for their study [2].

Observation of elegant physical phenomena in low-dimensional systems has enticed scientists to actively explore possibilities of other two-dimensional (2D) materials with outstanding characteristics. In this regard, monolayer MoS$_2$, belonging to the family of layered transition metal dichalcogenides, has been synthesized recently through mechanically cleaving bulk MoS$_2$, a layered material studied since the 1960s and which is held together by weak van der Waals interaction. Just as graphene, MoS$_2$ atoms are arranged hexagonally and it exhibits novel correlated electronic phenomena ranging from insulator to superconductor and is still flat enough to confine electrons so that charge flows quickly leading to a relatively high mobility that is promised by electronic and optical properties [3].

The monolayer MoS$_2$ has recently attracted great interest because of its potential applications in 2D nanodevices [4, 5], owing to the structural stability and lack of dangling bonds [6]. The monolayer MoS$_2$ is a direct gap semiconductor with an optical bandgap of 1.8 eV [4], and can be easily synthesized by using scotch tape or lithium-based intercalation [4–7]. The mobility of the monolayer MoS$_2$ can be at least 217 cm$^2$V$^{-1}$s$^{-1}$ at room temperature using hafnium oxide as a high-$\kappa$ gate dielectric, and the monolayer MoS$_2$ transistor shows the room temperature current on/off ratios of $10^8$ and ultralow standby power dissipation [4]. Recently, the MoS$_2$ nanoribbons have been obtained by using the electrochemical method [8]. The experimental achievements triggered the theoretical interests on the physical and chemical properties of monolayer MoS$_2$ nanostructures to reveal the origins of the observed electrical, optical, mechanical, and magnetic properties, and guide the design of novel MoS$_2$-based devices.

Thermodynamic quantities such as the electronic compressibility, the physical observable quantity most directly related to the energy and measures the stiffness of the system against changes in the density of electrons, is very powerful probe of exchange and correlation effects in interacting many-electron systems since they are intimately linked with the equation of state [9]. In an ordinary 2D electron gas corrections to the compressibility due to the correlation effects omitted in Hartree-Fock (HF) approximations are relatively small. Ilani et al. [10] performed a thermodynamic investigation of the 2D electron system measuring the compressibility. They found that the compressibility of the metallic phase largely follows Hartree-Fock theory, and that it is spatially homogeneous. Similar results were also reported by Dultz and Jiang [11] for the thermodynamic signature of the metal-insulator transition. Moreover, compressibility measurements of 2D electron gas systems have been carried out [12] and it is found qualitatively that Coulomb interactions affect the compressibility at sufficiently low electron density or strong coupling constant region. Recently, the local compressibility of graphene has also been measured [13] by using a scannable single-electron transistor, and theoretically the compressibility was calculated [14].

In recent years, because of the important and novel physical properties found in both theoretical and technological applications, there has been a large amount of theoretical and experimental studies on the transport...
properties of 2D electron systems. Although the basic mechanism and the existence of a quantum phase transition is still a matter of on-going debate, experiments have amassed a wealth of data on the transport properties of the 2D electron systems in the metallic state. As a function of the interaction strength, which is characterized by the ratio \( r_s = (\pi n a_B^2)^{-1/2} \) in which \( a_B \) is the Bohr radius of the Coulomb energy to Fermi energy, many novel correlated ground states have been predicted such as a paramagnetic liquid \( (r_s < 26) \), ferromagnetic liquid \( (26 < r_s < 35) \) and Wigner crystal \( (r_s > 35) \) [15, 16].

A ferromagnetic [17] behavior has also been reported in MoS\(_2\) and it has been related to edges or to the existence of defects [18]. The magnetic properties of MoS\(_2\) nanoribbons are not negligible. Furthermore, the effect of Coulomb interactions on the low-energy band structure of MoS\(_2\) using an effective two-band model Hamiltonian has been recently studied [19] and they showed that a large conduction band spin splitting and a spin dependent Fermi velocity are generated due to the Coulomb interaction.

The purpose of this paper is to study the transport properties such as band gap renormalization and charge compressibility of monolayer MoS\(_2\) systems. In this work, we present calculations of the zero temperature electronic compressibility and the quantum magnetic phase transition of disorder-free monolayer MoS\(_2\) based on a two-band continuum model. We show that the compressibility of a monolayer MoS\(_2\) is remarkably different from the two-dimensional electron gas and also from graphene monolayer and its behavior is not a monotonic function of the charge (electron or hole) density. To investigate the magnetic phase of the ground-state in the Hartree-Fock approximation, we use the Stoner exchange model which is the exchange interaction. To study the effect of electron-electron interactions, we use a model which includes both intra-valley (long range) and inter-valley (short range) interactions as introduced by Roldan et al [21]. We consider the interaction of quasiparticles by using the leading diagram approximation, which is the exchange interaction.

In this sense, the interacting Hamiltonian reads as

\[
\hat{V}_{\text{intra}} = \frac{1}{2S} \sum_{\mathbf{k},\mathbf{k}',\mathbf{q},\beta\neq\alpha} v_{q,k} \psi^\dagger_{k-q,\alpha}\psi^\dagger_{k-q',\beta}\psi_{k',\beta}\psi_{k,\alpha} \\
\hat{V}_{\text{inter}} = \frac{U}{2S} \sum_{\mathbf{k},\mathbf{k}',\mathbf{q},\beta,\beta'} v_{q,k} \psi^\dagger_{k-q,\alpha}\psi^\dagger_{k+\mathbf{q},\beta}\psi_{k',\beta}\psi_{k,\alpha} 
\]

where \( \mathbf{s} = -s \) and \( \tau = -\tau \) indicating the spin and valley indices, respectively. In order to account screening and to avoid any divergence within mean-field theory in systems with long-range interactions, we use an interaction potential including Thomas-Fermi screening

\[
v_q = \frac{2\pi e^2}{e_0 (|q| + \lambda q_{\text{TF}})}
\]

where \( e_0 \) is the effective dielectric constant and \( q_{\text{TF}} = 2\pi e^2 D(\epsilon_F)/e_0 \) is Thomas-Fermi screening wave vector in which \( D(\epsilon_F) = (g/2\pi)|kdkd\epsilon| \) is the density of states at the Fermi energy, i.e. \( k = k_F \). Parameter \( \lambda \) indicates the contribution of the Thomas-Fermi screening and changes between zero and unity. Notice that the Thomas-Fermi wave vector is much larger than a typical Fermi wave vector due to the large band-energy effective mass that occurs in MoS\(_2\). Here \( g \) indicates the degeneracy of each energy level and \( U = U_{4d} \times S \) where \( U_{4d} \) is the Hubbard repulsion coefficient which mostly originates from 4d orbitals of Mo atoms [21] and \( S = 3\sqrt{3}/2a_0^3 \) is the unit cell area.

II. THEORY AND METHOD

Two-band single particle Hamiltonian of the monolayer MoS\(_2\), neglecting the trigonal warping and the spin-orbit coupling of the conduction band, is given by [20]

\[
\mathcal{H}_0 = \sum_{\mathbf{k},\tau,\sigma,\alpha} \psi^\dagger_{\mathbf{k},\tau,\sigma,\alpha}\mathcal{H}_{\alpha\beta}(k,\tau)s_{\alpha\beta}\psi_{\mathbf{k},\tau,\sigma,\beta} \\
\mathcal{H}(k,\tau) = \frac{\Delta}{2} \sigma_z + \lambda_{soc} \tau s \frac{1 - \sigma_z}{2} + t_0 a_0 s k \cdot \sigma_z \\
+ \frac{\hbar^2 |k|^2}{4m_0} (\alpha + \beta \sigma_z)
\]

where \( a_0 = 0.184\text{nm} \), \( \lambda_{soc} = 0.08eV \), \( \Delta = 1.9eV \), \( t_0 = 1.68eV \), \( \alpha = 0.43 \), and \( \beta = 2.21 \). The field operators in the Hamiltonian are defined as \( \psi_{k,\tau,\sigma} = (a^\dagger_{k,\tau,\sigma}b^\dagger_{\mathbf{k},\tau,\sigma}) \) in which \( a^\dagger_{k,\tau,\sigma} \) and \( b^\dagger_{\mathbf{k},\tau,\sigma} \) are creation operators in the pseudospin space. To study the effect of electron-electron interactions, we use a model which includes both intravalley (long range) and inter-valley (short range) interactions as introduced by Roldan et al [21]. We consider the interaction of quasiparticles by using the leading diagram approximation, which is the exchange interaction.

The rest of this paper is organized as follows. In the next section we outline our theoretical approach to calculate the ground-state energy of MoS\(_2\) systems within the Hartree-Fock from which the quasiparticle excitations are obtained. The essential ingredients of our theoretical framework are the effective inter- and intra-valley electron-electron interactions where their discussions are appeared in Sec.II. Our numerical results for the bandgap renormalization and charge compressibility of both the electron and hole doped systems are presented in Sec.III. We conclude in Sec.IV with a brief summary of our main results.

A. Mean-Field Hamiltonian

The simplest approach to study an interacting electron gas in jellium approximation is the mean-field Hartree-Fock method, which the Slater determinant wave function minimizing the ground-state energy. In unpolarized jellium, the common solution is a paramagnetic state with spin symmetry. In 1962, Overhauser [22] proved
FIG. 1. (color online) Bandgap renormalization as a function of charge carrier density for the electron and hole doped cases for the varies dielectric constants. Note that the band gap does not depend on $U_{4d}$. The band gap renormalization decreases with increasing of the charge density and becomes smaller for a higher screening case. (b) in the hole doped case, The band gap renormalization shows a discontinuous function of the density associated an energy value equal to the $2\lambda_{soc}$.

FIG. 2. (color online) Charge compressibility, defined by $(n^2\kappa)^{-1} = \partial \mu / \partial n$ with respect with $3\sqrt{3}a_0^2U_{4d}/80000\hat{A}^2$ where $\mu$ is the chemical potential for (a) the electron and (b) hole doped cases as a function of the charge density for the different values of the dielectric constant. The decrease in $\partial \mu / \partial n$ with density is a consequence of the difference between hyperbolic and parabolic dispersion relation. We see that $\partial \mu / \partial n$ is positive and enhanced by exchange interactions and behaves non symmetric with respect to the particle-hole exchange. Notice that the charge compressibility behaves non-monotonically at very low electron or hole density.

that the Hartree-Fock solution of electron gas systems is unstable with respect to spin and charge fluctuations at any density. The global minimum energy state within the Hartree-Fock is a spontaneously broken symmetry state [23].

The band eigenstates on the positive and negative energy bands have their pseudospins either align or opposite to the direction of the momentum [24–26]. Therefore, the
The space in which the Hamiltonian is diagonalized is based on an electron ($c_k$) and hole ($v_k$) operators and \( (c^\dagger_{k,\tau s}, v^\dagger_{k,\tau s}) = (a^\dagger_{k,\tau s}, b^\dagger_{k,\tau s})\mathcal{U} \) where \( \mathcal{U} \) is a unitary matrix which diagonalize the single particle Hamiltonian given by \( \mathcal{U} = (|\psi_+\rangle, |\psi_-\rangle) \). We thus have

\[
\begin{align*}
    a_{k,\tau s} &= \frac{-(t_0a_0)\tau k e^{-i\phi}}{\sqrt{(t_0a_0)^2k^2 + D^2_\pm}}(\text{sign}(D_+)c_{k,\tau s} + \text{sign}(D_-)v_{k,\tau s}) \\
    b_{k,\tau s} &= \frac{1}{\sqrt{(t_0a_0)^2k^2 + D^2_\pm}}(|D_+|c_{k,\tau s} + |D_-|v_{k,\tau s})
\end{align*}
\]

Using above relations together with \( \langle \psi_0 | c^\dagger_{k,\tau s} c_{k,\tau s} | \psi_0 \rangle = n_{k,\tau s}^c \), \( \langle \psi_0 | v^\dagger_{k,\tau s} v_{k,\tau s} | \psi_0 \rangle = n_{k,\tau s}^v \) and \( \langle \psi_0 | c^\dagger_{k,\tau s} v_{k,\tau s} | \psi_0 \rangle = \langle \psi_0 | v^\dagger_{k,\tau s} c_{k,\tau s} | \psi_0 \rangle = 0 \), it would be easy to find the density matrix as

\[
\rho_{a_\alpha}(k, \tau s) = \frac{n_{k,\tau s}^c}{(t_0a_0)^2k^2 + D^2_\pm} + \frac{n_{k,\tau s}^v}{(t_0a_0)^2k^2 + D^2_\pm}, \quad \rho_{a_\beta}(k, \tau s) = \frac{D^2_+ n_{k,\tau s}^c}{(t_0a_0)^2k^2 + D^2_\pm} + \frac{D^2_- n_{k,\tau s}^v}{(t_0a_0)^2k^2 + D^2_\pm}
\]

Consequently, the mean-field Hamiltonian can be written as

\[
\mathcal{H}_{MF} = B_0^*(k)\sigma_0 + B^{\tau*}(k) \cdot \sigma_\tau
\]
The low-energy Hamiltonian is no longer valid and a function over ally originate from the integration over the whole valence 0.

\[ B_0^+(k) = \frac{1}{2} \lambda_{soc} \gamma^s + \frac{\hbar^2 k^2}{4m_0} \alpha - \frac{1}{2} \int \frac{d^2 k'}{(2\pi)^2} v_{k-k'} (n_{k',\tau}^v + n_{k',\tau}^s) + U \int \frac{d^2 k'}{(2\pi)^2} \{ n_{k',\tau}^v + n_{k',\tau}^s \} \]

\[ B_0^-(k) = \frac{\Delta - \lambda_{soc} \gamma^s}{2} + \frac{\hbar^2 k^2}{4m_0} \beta - \frac{1}{2} \int \frac{d^2 k'}{(2\pi)^2} v_{k-k'} \left\{ \left( t_0 a_0 \right)^2 \gamma^2 - D_+ \left( t_0 a_0 \right)^2 \gamma^2 + D_+ \right\} n_{k',\tau}^v + \frac{\left( t_0 a_0 \right)^2 \gamma^2 - D_+ \left( t_0 a_0 \right)^2 \gamma^2 + D_+ n_{k',\tau}^s \}

\[ B_0^y(k) = (t_0 a_0) k \sin \phi + \int_{k_F}^{k_F} \int_{0}^{2\pi} \frac{k'dk'\phi'}{(2\pi)^2} v_{k-k'} \left( t_0 a_0 \right)^2 \gamma^2 + D_+ \sin \phi' + \int_{0}^{k_F} \int_{0}^{2\pi} \frac{k'dk'\phi'}{(2\pi)^2} v_{k-k'} \left( t_0 a_0 \right)^2 \gamma^2 + D_+ \cos \phi' + \int_{0}^{k_F} \int_{0}^{2\pi} \frac{k'dk'\phi'}{(2\pi)^2} v_{k-k'} \left( t_0 a_0 \right)^2 \gamma^2 + D_+ \sin \phi' \]

Here \( k_c \) indicates ultraviolet cutoff for larger than that the low-energy Hamiltonian is no longer valid and a typical value of the \( k_c = 1/a_0 \), whereas we set \( k_c = 0.5/a_0 \) to be more precise based on the comparison between the electron dispersion relation calculated by the Hamiltonian, Eq. (1), and those results obtained by \( ab initio \) band structure [27]. Notice that we ignore two infinite terms, namely \( I_1 = \int_{0}^{k_F} \{ kdk \} \) and \( I_2 = \int_{0}^{k_F} \int_{0}^{2\pi} \{ v_{k-k} kdk \} \) in the \( B_0 \) term which they actually originate from the integration over the whole valence bands per each spin component. Moreover, the integration over \( B_0 \) yields as

\[ \int_{0}^{k_F} B_0^+(k) kdk = \frac{1}{4} \lambda_{soc} \gamma^s k_F^2 + \frac{\hbar^2 \alpha}{16m_0} k_F^4 + \frac{U}{8\pi} k_F^2 k_F^2 \]

\[ \int_{0}^{k_F} B_0^y(k) kdk = \frac{1}{2} \int_{0}^{k_F} \int_{0}^{2\pi} \frac{kdk'k'dk'\phi'}{(2\pi)^2} v_{k-k'} \]

B. Ground-state of the electron doped system

To calculate the ground-state energy within the Hartree-Fock approximation, we do need to evaluate \( k_F \) which is the Fermi wave vector of two spin components at each valley where for the electron doped case they are the same, \( k_F = k_F (1 + s c)^{1/2} \), however for a hole doped case, they differ from each other. The Fermi wave vector given by \( k_F = \sqrt{4\pi n/g} \) where \( g \) stands for the degeneracy of the band structure which is equal to 4 for the electron and highly hole doped cases while for the low hole doping it is equal to 2. At zero temperature and electron doped case, the set of Eq. (11) can simplify as

\[ \int_{0}^{k_F} B_0^+(k) kdk = \frac{1}{4} \lambda_{soc} \gamma^s k_F^2 + \frac{\hbar^2 \alpha}{16m_0} k_F^4 + \frac{U}{8\pi} k_F^2 k_F^2 \]

C. Ground-state of the hole doped system

In a similar way, corresponding relations in the hole doped case can be found as
It should be noted that in the hole doped case there are two Fermi wave vectors $k_{F1}$ and $k_{F2}$ which can be calculated from $\varepsilon_{k_{F1},++} = \varepsilon_{k_{F2},--} = \varepsilon_F$ and $\varepsilon_{k_{F2},+-} = \varepsilon_F$, respectively, where we have used non-interacting energy dispersion. Note that $k_{F2} = 0$ when the Fermi energy is located in the spin splitting energy range and does not intersect with spin down (up) band around the $K$ ($K'$) point.

\[
\begin{align*}
B_0^s(k) &= \frac{1}{2} \lambda_{soc} \tau s + \frac{\hbar^2 k^2}{4m_0} \alpha + \frac{1}{2} \int_{k_F}^{kp_{s}} \int_{0}^{2\pi} \frac{k'dk'd\phi'}{(2\pi)^2} v_{k'k'}^{-1} - \frac{U}{4\pi} k_{F}^2 \\
B_0^x(k) &= \frac{\Delta - \lambda_{soc} \tau s}{2} + \frac{\hbar^2 k^2}{4m_0} \beta + \frac{1}{2} \int_{0}^{k_{F}} \int_{0}^{2\pi} \frac{k'dk'd\phi'}{(2\pi)^2} v_{k'k'}^{-1} (t_0 a_0) k'^2 - D^2 - \frac{1}{2} \int_{0}^{k_{F}} \int_{0}^{2\pi} \frac{k'dk'd\phi'}{(2\pi)^2} v_{k'k'}^{-1} (t_0 a_0) k'^2 + D^2 \\
B_0^y(k) &= (t_0 a_0) k \cos \phi - \int_{0}^{k_{F}} \int_{0}^{2\pi} \frac{k'dk'd\phi'}{(2\pi)^2} v_{k'k'}^{-1} (t_0 a_0) k' D_+ - \frac{1}{2} \int_{0}^{k_{F}} \int_{0}^{2\pi} \frac{k'dk'd\phi'}{(2\pi)^2} v_{k'k'}^{-1} (t_0 a_0) k' D_- (2\pi)^2 \cos \phi' \\
B_0^z(k) &= (t_0 a_0) k \sin \phi - \int_{0}^{k_{F}} \int_{0}^{2\pi} \frac{k'dk'd\phi'}{(2\pi)^2} v_{k'k'}^{-1} (t_0 a_0) k' D_+ (2\pi)^2 \sin \phi'
\end{align*}
\] (14)

doped case, reads as

\[
\begin{align*}
\varepsilon_{tot}(n, \zeta, \epsilon_0, U) &= E_T + E_L \frac{N_T + N_L}{2} \\
E_s &= \frac{1}{2} \sum_{k\tau} \sum_{s, r,s} \varepsilon_{k\tau s} n_{k\tau s}^c d^2 k \\
N_s &= \frac{1}{2} \sum_{k\tau} n_{k\tau s}^c d^2 k = \frac{1}{2} \int_{0}^{k_{F}} \int_{0}^{2\pi} \varepsilon_{k\tau s} d^2 k
\end{align*}
\] (15)

where the total energy of the occupied state in the valence band is considered as the vacuum energy and we ignore its contribution in the energy per particle. At zero temperature and electron doped case we have

\[
\begin{align*}
\varepsilon_{tot}(n, \zeta, \epsilon_0, U) &= \sum_{k\tau} \int_{0}^{k_{F}} \varepsilon_{k\tau s} d^2 k \\
N_s &= \frac{1}{2} \int_{0}^{k_{F}} \int_{0}^{2\pi} \varepsilon_{k\tau s} d^2 k
\end{align*}
\] (16)

Furthermore, for the low hole doped case one gets

\[
\begin{align*}
\varepsilon_{tot}(n, \zeta, \epsilon_0, U) &= - \sum_{k\tau} \int_{0}^{k_{F}} \varepsilon_{k\tau s} d^2 k \\
N_s &= \frac{1}{2} \int_{0}^{k_{F}} \int_{0}^{2\pi} \varepsilon_{k\tau s} d^2 k
\end{align*}
\] (17)

Finally, since the exchange interaction between itinerant electrons tends to cause a magnetic instability, the critical density [28] in which the paramagnetic-to-ferromagnetic Bloch phase transition [29] occurs can be obtained by criteria in which $\varepsilon_{tot}(n_{cr}, 0, \epsilon_0, U_{ad}) = \varepsilon_{tot}(n_{cr}, 0, \epsilon_0, U_{ad})$. Efforts to observe the ferromagnetic phase predicted by Bloch have likewise been frustrated by the difficulty of achieving low values of the charge density. The closest thing to an experimental observation of this transition has come so far from experiments in the 2D electron gas.
in a high magnetic field. Under appropriate conditions the magnetic field suppresses not only the kinetic energy, but also the correlation energy. This leaves the exchange energy master of the field, and leads to a ferromagnetic transition. Here, we show that the such a transition takes place for a hole doped system much easier than an electron doped case in the absence of the magnetic field.

III. NUMERICAL RESULTS

We now turn to our main numerical results. The ground-state properties of the MoS$_2$ are completely determined by the total density $n$, by the intra-valley interaction $U_{4d}$ and by the media dielectric constant, $\epsilon_0$. Here, we set $\lambda = 1$, otherwise we determine its value specifically.

The calculation of $\mu$ and of $\partial \mu/\partial n$ is carried out by performing numerically the first and the second derivatives, respectively, of the ground-state energy, which, in turn, is known only numerically from Eqs. (12) and (14).

Fig. 1 shows the BGR for the various dielectric constants as a function of the charge density. The BGR does not depend on $U_{4d}$. The BGR decreases with increasing of the charge density and becomes smaller for a higher screening case. It is a smooth and monotonic function in the electron doped system shown in Fig. 1(a). However, in the hole doped case, Fig. 1(b) we have obtained a discontinuous function of the density associated an energy value equal to the $\lambda_{soc}$ and the BGR tends to a constant weight increasing the hole density.

In Fig. 2, we report Hartree-Fock theory results in the inverse thermodynamic density of states $\partial \mu/\partial n$ with respect to $3\sqrt{3}a_0^2U_{4d}/80000\,\text{A}^2$ as a function of the charge density. The decrease in $\partial \mu/\partial n$ with density is a consequence of the difference between hyperbolic and parabolic dispersion. We see that $\partial \mu/\partial n$ is positive and enhanced by exchange over the density range covered in this plot. Since the compressibility involves only occupied states, its behavior is not symmetric with respect to particle-hole exchange. Notice that the charge compressibility behaves non-monotonically at very low electron or hole density. In Ref. [30] and Ref. [31] a non-monotonic behavior were also found in a bilayer graphene system within the Hartee-Fock and random phase approximation, respectively, and the change in the sign of the inverse thermodynamic density of states predicted in very low density.

We also examine our results by considering a small $\lambda = 0.01$ value in which the Coulomb interaction is much larger than screened potential in particular at the long wavelength limit. The inverse thermodynamic density of states with respect to $3\sqrt{3}a_0^2U_{4d}/80000\,\text{A}^2$ as a function of the electron density is shown in Fig. 3 where $\lambda = 0.01$. The results are qualitatively the same as results depicted in Fig. 2, however the value of the physical values are changed quantitatively. We find that the change in the sign of the inverse thermodynamic density of states occurs in a larger density with decreasing the value of the $\lambda$.

To calculate the magnetic phase transition, we investigate the condition for which $\varepsilon_{tot}(n, 1, \epsilon_0, U_{4d}) = \varepsilon_{tot}(n, 0, \epsilon_0, U_{4d})$ is satisfied by giving $n$, $U_{4d}$ and $\epsilon_0$ parameters. Figure 3(a) shows the magnetic phase diagram at given charge density, $n = 5 \times 10^12\,\text{cm}^{-2}$. From this comparison one arrives at the conclusion that in MoS$_2$, the paramagnetic liquid has the lowest energy for $U_{4d} < 3\text{eV}$ for electron doped case, while the ferromagnetic liquid has the lowest energy in the larger value of the $U_{4d}$ in a wide range of the dielectric constant. More-
over, the critical value of the charge density in which the phase transition is occurred is plotted as a function of the intervalley interaction for both electron and hole cases in Fig. 3(b). The results suggest that the system with hole charge carrier can easily go to the ferromagnetic phase in comparison with a situation in which the charge carrier is the electron. The reason for this discrepancy is that, in the low hole-doped case, the density of states is twice smaller than those of the electron doped system, owing to the spin-splitting in the valence band. Consequently, the screening effect is weaker for the holes which provides a stronger impact of the interaction to induce a ferromagnetic phase for holes. Moreover, the spin-valley coupling of the holes results in a valley-ferromagnetism together with a spin-polarized magnetic phase. Therefore, the Hartree-Fock calculation predicts a spin-valley-polarized ground-state for the holes while that of electrons is just spin-polarized in monolayer MoS$_2$.

It turns out that the Bloch transition, a ferromagnetic ground-state, is not quantitatively accurate in the Hartree-Fock approximation. In order to obtain accurate ground-state energy, a renormalized Hamiltonian for low-Hartee-Fock approximation is not quantitatively accurate in the magnetic ground-state, is not quantitatively accurate in the Hartree-Fock approximation, we use the Stoner exchange model in which it is assumed that the system is partially spin polarized. Our numerical results predict that the system with hole charge carriers can easily go to the ferromagnetic phase in comparison with a situation in which the charge carriers are electrons.

We note that, although the Hartree-Fock method has provided valuable information about the relative stability of the simplest phases of the electronic structure of the MoS$_2$, we clearly cannot claim to have achieved a complete understanding of the magnetic phase diagram of the system. The occurrence of transitions between states of different symmetry indicates that the ground-state energy of the system is a nonanalytic function of parameters, namely homogenous charge density, the knowledge of the energy functional appropriate to an infinitesimally polarized electron liquid are needed.

IV. SUMMERY

In conclusion, we have studied the electronic compressibility of a monolayer MoS$_2$ within the Hartree-Fock approximation and have found a behavior that is remarkably different from the two-dimensional electron gas and also from graphene monolayer. We have shown that the inverse compressibility is not a monotonic function of the charge (electron or hole) density and it is due solely to intrinsic electronic interactions. The change of the trend of the inverse compressibility was numerically calculated and the critical value of the charge density depends on screening procedure that we have used in our model. We have also neglected the trigonal warping term, which might be important at very high densities of holes. In order to investigate the magnetic phase of the ground state in the Hartree-Fock approximation, we use the Stoner exchange model in which it is assumed that the system is partially spin polarized. Our numerical results predict that the system with hole charge carriers can easily go to the ferromagnetic phase in comparison with a situation in which the charge carriers are electrons.

We note that, although the Hartree-Fock method has provided valuable information about the relative stability of the simplest phases of the electronic structure of the MoS$_2$, we clearly cannot claim to have achieved a complete understanding of the magnetic phase diagram of the system. The occurrence of transitions between states of different symmetry indicates that the ground-state energy of the system is a nonanalytic function of parameters, namely homogenous charge density, the averaged dielectric constant, the spin degree of freedom, and finally the Hubbard repulsion coefficient.

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