Strong electron-lattice coupling as the mechanism behind charge density wave transformations in transition-metal dichalcogenides

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We consider single band of conduction electrons interacting with displacements of the transitional ions. In the classical regime strong enough coupling transforms the harmonic elastic energy for an ion to the one of the well with two deep minima, so that the system is described in terms of Ising spins. Inter-site interactions order spins at lower temperatures. Extension to the quantum regime is discussed. Below the CDW-transition the energy spectrum of electrons remains metallic because the structural vector $\mathbf{Q}$ and the FS sizes are not related. Large values of the CDW gap seen in the tunneling experiments correspond to the energy of the minima in the electron-ion two-well complex. The gap is defined through the density of states (DOS) inside the electronic bands below the CDW transition. We focus mainly on electronic properties of transition-metal dichalcogenides.

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I. INTRODUCTION

Origin of charge density waves (CDW) in the transition-metals dichalcogenides (TMDC) is subject of debates since their discovery in the early 70's [1]. At the time, the most popular theoretical scenario was the so-called "nesting", the congruency of two or more Fermi surfaces (FS) separated by a vector $\mathbf{Q}$ in the momentum space. Interactions with the momentum transfer $\mathbf{Q}$ would lead to the CDW instability (with $\mathbf{Q}$ becoming the structural vector) and to the opening of energy gaps on FS.

The alternative explanation [2] ascribes the structural instability to the presence of saddle points in the electronic spectrum near the Fermi energy. The logarithmic singularities in the electronic density of states (DOS) at the saddle points favor instabilities with the momentum transfer, $\mathbf{Q}$ connecting the two saddle points. The mechanism also leads to the energy gaps in the electron spectrum.

Subsequent experiments and band structure calculations for real materials gave no support to either of the two concepts. The CDW transition does not affect properties of dichalcogenides any noticeable. Materials remain metallic below the transition temperature, T_{CDW}. Superconductivity in $2H$-TaSe$_2$, $2H$-TaS$_2$ and $2H$-NbSe$_2$ takes place on the background of the CDW phase. The CDW gap values ~ 0.1 eV surprisingly large in comparison with the values of transition temperatures, $T_{\mathrm{CDW}}(\mathrm{Ta}) = 122$ K and $T_{\mathrm{CDW}}(\mathrm{Nb}) = 33.5$ K, were observed via the dI/dV characteristics in the tunneling experiments [3]. The gap of such order of magnitude is noticeable in the infrared data [4] ($2H$-TaSe$_2$) even close to the transition temperature.

The phenomenological analysis in [5] revealed the short coherence length in the CDW phase, $\xi_0 \sim 3 - 10$ Å, thus implying the important role of fluctuations.

The density functional calculations [6] ($2H$-NbSe$_2$) have shown that the contribution from the nested pieces of FS into the charge susceptibility is negligible at the expected value of the vector $\mathbf{Q}$, although, indeed, the ground state of the system at $T = 0$, according to [6], is the CDW phase.

It was well known since 1958 that at the strong enough e-ph coupling the square of renormalized phonon frequency turns out negative, thus signaling instability of the lattice [7]. In [8] through the example of $1T$-TaS$_2$, it was demonstrated that CDW transitions in the transition-metal dichalcogenides can be driven by the Migdal's instability [7]. The new tinge added to this concept in [8] was that dispersion of the renormalized (imaginary) soft mode can become strongly peaked near the structural vector of instability, $\mathbf{Q}$ if the e-ph matrix element depends on the transferred momentum.

There is no small physical parameter in the problem [7]. Correspondingly, there are no other means in [8] to discuss electronic properties of $2H$-TaSe$_2$ and $2H$-NbSe$_2$ beside numerical calculations.

As it was already mentioned above, the nesting scenario and that one of Ref. 2 both contradict to the experimental data [3, 4] and to their analysis and the interpretation [5, 8]. In spite of that, the two concepts are commonly used for interpretation of results even in recent ARPES experiments (see, e.g., [9, 10]).

We address peculiarities of transition-metal dichalcogenides from the point of view differing from [8]. We argue that instead of development of the Migdal instability in the soft mode scenario [8] for the *propagating* phonon mode, the CDW instability may realize itself in the two stages. Namely, at first, strong e-ph interactions bring electrons and ions close together in kind of a polaronic effect similar to the one first discussed for V$_3$Si in [11]. The potential in which the ion moves becomes anharmonic. At a strong enough e-ph coupling the potential possesses two minima, so that the system can be described in terms of Ising spins. The subsequent ordering of the local sites at a lower temperature occurs due to inter-site interactions.

In Ref. 11 electron-lattice interactions were limited to the interaction of electrons with single dispersionless (Einstein) optical mode. In the approach below conduction electrons interact with arbitrary ionic displacements. Strength of the intersite interactions and the value of contributions into the local elastic potential are separately evaluated.

"Trapping" of the electronic cloud near an ion by the elastic field is deemed responsible for the main energy gains and pre-determines, whereby, by the order of magnitude, the energy scale of the CDW gap. According to our estimates, the wells' minima are deep ($\sim$ few tenths of 1 eV). Thereby, the Kondo-like regime of quantum tunneling that was the subject of the main concern in [11] seems to be of no relevance to dichalcogenides, at least at the temperatures of interest. We focus in the following on properties of the electronic sub-system.

II. CHOICE OF THE MODEL

Before proceeding further, we briefly summarize the information pertaining to the CDW transitions in TMDC.

Symmetry of the order parameters governing the transition was discussed in [5, 12]. The lattice superstructure below T_{CDW} [1] is formed by the triple-$\mathbf{Q}$ modulations of the ionic positions along the three symmetry axes in the hexagonal *2H*-phase. The $\mathbf{Q}$-vector may be incommensurate, but even then $\mathbf{Q}$ remains very close to $\vec{a}^*/3$ (here $a^* = 4\pi/\sqrt{3}a$).

It was perceived already in the early 70's [13] that the structural changes in $2H$-NbSe$_2$ are related to displacements of the niobium ions. Correspondingly, in what follows, we choose a simplified model and consider only shifts of the transition-metals ions (Nb or Ta) along each of these three symmetry lines. The dramatic softening of the longitudinal acoustic mode with $\mathbf{Q}$ about $\vec{a}^*/3$ was recently observed in [14]. Note, in passing, that the optical modes and the longitudinal acoustic branch of the same Σ_1- symmetry are actually linearly coupled near point $\vec{a}^*/3$ of the Brillouin Zone (BZ). We return to this later to show that softening of the optical mode is accompanied by softening of the acoustic phonon, and vice versa.

Transition-metals dichalcogenides are layered compounds with the weak Van der Waals coupling between the layers. We restrict ourselves by the quasi-two-dimensional properties (Q2D) of a single layer.

We consider a single isotropic band of electrons interacting strongly with displacements of the transition-metal ions. Implicitly, the band is assumed to be predominantly of the 4f (Nb) - or 5f (Ta) - character.

In the model [8] the "bare" frequency of the *propagating phonon mode*, $\omega_0^2(\mathbf{k})$ is renormalized by the polarization operator [15] (with the *e-ph* matrix element $g(\mathbf{p}, \mathbf{p} + \mathbf{k})$ is peaked at $\mathbf{k} \approx \mathbf{Q}$). Unlike [8], our attention is concentrated on the *local environment* of the single ion. In this respect, as we discuss later, our model shows some features common to the Holstein model [16].

For a heavy ion one may expect that quantum effects are not crucial for properties of the lattice, at least, at not too low a temperature. The temperature of the (incommensurate) transition in $2H$-TaSe$_2$, $T_{\text{CDW}} = 122$ K [1] is rather high and, in the first approximation, one can neglect the kinetic energy of the Ta ions.

With the notations u_i for a displacement of the single ion at the point R_i the "bare" elastic matrix is: $U(R_i - R_j)u_iu_j$. At $i = j$ it is merely the potential energy of the oscillator:

$$U(R_i - R_j)u_iu_j \Rightarrow \frac{1}{2}M\omega_0^2u_i^2 = \frac{1}{2}ku_i^2 . \tag{1}$$

Interactions with electrons change the elastic matrix. We calculate the contribution to the elastic energy that is due to interactions of electrons with arbitrary static displacements.

With the Hamiltonian for the *e-ph* interaction in the form

$$\hat{H}_{e-ph} = \sum_i gu_i\hat{\psi}^+(R_i)\hat{\psi}(R_i) \tag{2}$$

the energy of the coupled electron-lattice system $E(u_1...u_N; g)$ can be calculated from the equation:

$$\frac{\partial E(u_1...u_N)}{\partial g} = \sum_i u_in(R_i) , \tag{3}$$

where $n(R_i) = \langle\hat{\psi}^+(R_i)\hat{\psi}(R_i)\rangle$ is the number of electrons per unit cell at the point R_i. In terms of the electronic Green function (at $T = 0$, [15]), $G_{\alpha\beta}(R, t; R', t') = -i\langle T(\psi_\alpha(R_i, t)\hat{\psi}_\beta^+(R', t'))\rangle$, one has: $n(R_i) = -2iG(R, t; R, t + \delta)$. (The Green function is diagonal in the spin indices: $G_{\alpha\beta}(R, t; R', t') = -i\delta_{\alpha\beta}G(R, t; R', t')$).

III.   COUPLED ELECTRON-LATTICE SYSTEM IN THE CLASSICAL REGIME

At static displacements, one needs to know only the frequency component, $G(R, R'; \omega)$:

$$G(R, t; R', t') = \int \frac{d\omega}{2\pi} G(R, R'; \omega) \exp(-i\omega(t - t')) . \tag{4}$$

Re-arrange the power expansion of $G(R, R'; \omega)$ in u_i as:

$$G(R, R'; \omega) = G_0(R - R'; \omega) + \sum_i G_0(R - R_i; \omega)g\bar{u}_iG_0(R - R_i; \omega) \tag{5}$$

$$+ \sum_{i \neq k} G_0(R - R_i; \omega)g\bar{u}_iG_0(R_i - R_k; \omega)g\bar{u}_kG_0(R_k - R'; \omega) + ...$$

The *e-ph* contributions in *all powers* in g are now summed first for the single site: $u_i \Rightarrow \bar{u}_i$. Each of $\bar{u}_i, \bar{u}_k, ...$ in Eq. (5) stands for the "dressed" local deformation at the corresponding site, R_i, R_k, ..., and is determined by the relation:

$$baru_i = u_i + u_iG_0(R_i = R_i; \omega)g\bar{u}_i . \tag{6}$$

The free Green function, $G_0(R_i = R_i; \omega)$ equals [15]:

$$G_0(R_i = R_i; \omega) = \int \frac{d^2\bar{p}}{(2\pi)^2} \frac{1}{\omega - E(p) + E_F + i\mathrm{sign}(\omega)\delta} \ . \tag{7}$$

With the help of identity

$$\frac{1}{\omega - \xi + i\mathrm{sign}(\omega)\delta} = P\left(\frac{1}{\omega - \xi}\right) - i\pi\mathrm{sign}(\omega)\delta(\omega - \xi)$$

and assuming the electron-hole symmetry for $|\xi| = |E(p) - E_F|$, one obtains:

$$G_0(R_i = R_i; \omega) = -i\pi\nu(E_F)\mathrm{sign}(\omega) \ . \tag{8}$$

After trivial calculations, one finds the electronic contribution into the local elastic matrix at the site R_i, $E(u_i) = -2i \int_0^1 dg u_i G(R_i = R_i; t = t' + \delta; g)$:

$$E(u_i) = -\frac{W}{2\pi} \ln\left\{1 + [\pi\nu(E_F)gu_i]^2\right\} \ , \tag{9}$$

where W is the bandwidth. $E(u_i)$ is determined as the energy per one ion, $\nu(E_F)$ is the number of states at the Fermi level per unit cell: $\nu(E_F) = \left(\frac{m}{2\pi}\right) S_0$, where S_0 is the area of the 2D unit cell. $W\nu(E_F) = s$ is an insignificant model parameter, $s \sim 1$. We take $s = 2$.

The interaction between two sites, $E(u_i, u_k)$, is given by the second term in Eq. (5):

$$E(u_i, u_k) = u_i u_k(-i)g^2 \int \frac{d\omega}{2\pi} , G_0^2(R_{i,k}; \omega) \tag{10}$$

where $R_{i,k} \equiv |R_i - R_k|$.

The analytic form of $G_0(R_{i,k}; \omega)$ being cumbersome in 2D, for the estimate we use its asymptotic at $p_F R_{i,k} > 1$:

$$G_0(R; \omega) \Rightarrow i\nu(E_F)\sqrt{\frac{2\pi}{p_F R}} \exp\left\{i\mathrm{sign}(\omega)\left[\left(p_F + \frac{\omega}{v_F}\right)R - \frac{\pi}{4}\right]\right\} \ . \tag{11}$$

We obtain:

$$E(u_i, u_k) = u_i u_k g^2 \nu^2(E_F) p_F v_F \frac{\sin(2p_F R)}{(p_F R)^2} \ . \tag{12}$$

The total elastic energy of a single ion is the sum of Eqs. (1) and (9). Introducing:

$$g^2 = \left(\frac{M\omega_0^2}{2\pi\nu(E_F)}\right)\Lambda^2 \ , \tag{13}$$

$$\frac{\pi}{2}\left(M\omega_0^2\nu(E_F)\right) = \frac{1}{u_0^2} \ , \tag{14}$$

and the dimensionless notations for the ions' shifts, $\tilde{u}_i = (u_i/u_0)$, one writes down the local elastic energy in the following simple form:

$$U_{\mathrm{tot}}(u_i) = \frac{1}{\pi\nu(E_F)}\left[\tilde{u}_i^2 - \ln\left(1 + \Lambda^2\tilde{u}_i^2\right)\right] \tag{15}$$

Here Λ^2 is the square of the dimensionless e-ph coupling constant and u_0 determines the spatial scale of the local elastic potential. The energy scale $T^* = 1/\pi\nu(E_F) = W/2\pi$ is expressed through DOS in the electronic band. For $2H$-NbSe$_2$ the band calculations [17] gave $\nu(E_F) = 2.8$ states/eV per two bands. Here T^* is of the order of tenths of 1 eV.

At $\Lambda^2 > 1$ the potential $U_{\mathrm{tot}}(u_i)$ has two deep minima at $\tilde{u}_{+,-} = \pm\sqrt{1 - \Lambda^{-2}}$:

$$U_{\mathrm{tot}}(u_{+,-}) = (1/\pi\nu(E_F))\left[1 - \Lambda^{-2} - \ln\Lambda^2\right] \ . \tag{16}$$

At $\Lambda^2 < 1$ and temperatures below T^* $\tilde{u}_i \ll 1$ and $U_{\text{tot}}(u_i)$ can be written as:

$$U_{\text{tot}}(u_i) = (1/\pi\nu(E_F))\left\{\tilde{u}_i^2(1-\Lambda^2) + \frac{\Lambda^4}{2}\tilde{u}_i^4\right\} . \tag{17}$$

The quartic term in Eq. (17) is small, but the anharmonic contribution into the elastic energy is the necessary ingredient in the molecular field approach to a CDW transition (see, e.g., [18]).

Re-writing $p_F v_F$ as: $p_F v_F = (1/\pi\nu(E_F))(p_F^2 S_0/2)$, where $S_0 = (\sqrt{3}/4)a^2$ is the area of the triangular unit cell, Eq. (12) can be written down in the notations of Eqs. (13,14):

$$E(u_i, u_k) = \frac{1}{\pi\nu(E_F)}\left[\frac{\sqrt{3}}{4\pi^2}\Lambda^2\tilde{u}_i\tilde{u}_k\left(\frac{a}{R}\right)^2\sin(2p_F R)\right] . \tag{18}$$

The numerical factor in this expression shows that the inter-site interactions are weak compared to the on-site $U_{\text{tot}}(u_i)$.

At $\Lambda^2 > 1$ the model reduces to the model of interacting Ising spins:

$$\tilde{u}_{+,-}(i) \Rightarrow \sqrt{1-\Lambda^{-2}}\,\sigma_i, \quad \sigma_i = \pm 1 .$$

When $\Lambda^2 < 1$, the expressions for $U_{\text{tot}}(u_i)$ and Eq. (18) for $E(u_i, u_k)$ together complete formulation of the problem: in the classical regime the system is fully described by the partition function $Z(T,g)$:

$$Z(T,g) = \int(\Pi du_i)\exp\left[-\frac{1}{T}\sum_{i,k}U_{\text{tot}}(u_i, u_k)\right] , \tag{19}$$

where $U_{\text{tot}}(u_i, u_k) = U_{\text{tot}}(u_i) + E(u_i, u_k)$.

The phase transitions are habitually treated in the molecular field approximation (see, e.g., [18]). The method being not exact for short-ranged interaction; we do not discuss details of the CDW transitions itself.

For local properties one has for the partition function, $Z(T,g)$:

$$Z_i(T,g) = \int d\tilde{u}_i\exp\left\{-\frac{1}{\pi\nu(E_F)T}\left[\tilde{u}_i^2 - \ln(1+\Lambda^2\tilde{u}_i^2)\right]\right\} . \tag{20}$$

Scattering of electrons on the lattice displacements above T_{CDW} is characterized by the average $\langle g\bar{u}_i \rangle$ that enters the denominator of the Green function:

$$G^{-1}(R;\omega) = \omega - E(p) + E_F + \langle g\bar{u}_i \rangle . \tag{21}$$

From Eq. (6) it follows: $g\bar{u}_i = gu_i[1 - i\text{sign}(\omega)\pi\nu(E_F)gu_i]^{-1}$. In the normal phase terms that are odd in u_i can be omitted. In dimensionless variables:

$$g\bar{u}_i = i\text{sign}(\omega)\frac{1}{\pi\nu(E_F)}\frac{\Lambda^2\tilde{u}_i^2}{1+\Lambda^2\tilde{u}_i^2} . \tag{22}$$

At $\Lambda^2 < 1$ the imaginary part is: $G^{-1}(R;\omega)$ is $\langle g\bar{u}_i \rangle \cong i\text{sign}(\omega)\Lambda^2(\pi/2)\nu(E_F)T$. In the classical regime above T_{CDW} the resistivity of the system would be linear in T. In the opposite limit of $\Lambda^2 > 1$, $\tilde{u}^2 = \tilde{u}_{+,-}^2 = 1 - \Lambda^{-2}$, and the imaginary part is a constant of order of $1/\pi\nu(E_F)$. The entropy for the system of non-interacting Ising spins is finite.

In the ordered state with all ions occupying same minima, non-zero $g\bar{u}_i \neq 0$ stands together with the chemical potential:

$$g\bar{u}_i = \pm\frac{1}{\pi\nu(E_F)}\sqrt{\Lambda^2 - 1} . \tag{23}$$

So far, for simplicity of the arguments, it was tacitly implied that the order parameter $g\bar{u}_i \neq 0$ in Eq. (22) stands for the CDW transition with the structural vector $\mathbf{Q} = 0$. As in TMDC the $\mathbf{Q}$-vector is non-zero, the order parameter $g\bar{u}_i(Q)$ in Eq. (21) couples electronic states with the energies $E(p)$ and $E(p+Q)$.

In such a way, non-zero $g\bar{u}_i(Q)$ changes the energy spectrum and, hence, DOS in the vicinity of such paired points, but does it mainly for energies away from the Fermi level because in dichalcogenides the $\mathbf{Q}$-vector and sizes of the Fermi-surfaces are not related. Of course some Fermi-surfaces points may be affected at onset of the CDW order, as it is really observed in [9].

IV. DISCUSSION OF THE RESULTS

A. CDW instability: above and below T_{CDW}

It is interesting to discuss the relevance of the above model to the experimental results, in particular, for $2H$-TaSe$_2$.

First, recall that the non-linear potential (9) was derived for a single ion. For Eq. (9) to be meaningful, u_0 must be small compared to the lattice parameter, $a \approx 3.45$ Å. With the phonon frequencies, ω_0 for NbSe$_2$ typically in the range $10-20$ meV, is indeed small: $u_0 \leqslant 0.30 - 0.15$ Å. Similar estimates for $2H$-TaSe$_2$ give $u_0 \leqslant 0.2 - 0.1$ Å. This justifies the assumption. Experimentally, the superlattices shifts of cations are between 0.1 Å [1] and 0.5 Å [11] and, hence, have same order of magnitude as u_0, as it should be in the model of Ising spins.

In [4] the large CDW gaps ~ 90 meV and ~ 60 meV for $2H$-TaSe$_2$ and $2H$-NbSe$_2$, respectively, were derived from the tunneling non-linear current characteristics, dI/dV. Such values are in the right correspondence with the energy scale, $T^* = 1/\pi\nu(E_F)$ equal to $0.1 - 0.3$ eV, depending on the number of states per unit cell in the specific material (for NbSe$_2 \sim 2.8$ eV^{-1} per unit cell per two Nb bands [17]). So far, however, the CDW gap itself was rather vaguely defined. There, it was shown that the CDW with non-zero $\mathbf{Q}$ couples the electronic states with $E(p)$ and $E(p+Q)$. For the two symmetric points, $E(p-Q/2)$ and $E(p+Q/2)$, say, inside the energy band for the Fermi surface centered at the Γ-point, the energy spectrum in their vicinity is:

$$\bar{E}_{1,2}(p \pm Q/2) = E(p \pm Q/2) \pm |g\bar{u}_i(Q)| . \tag{24}$$

Eq. (24) defines the CDW gap as it appears in the $I - V$ characteristics which measure the energy dependence of DOS. The CDW gaps depend on the value of the parameter, $\Lambda^2 > 1$ as in Eqs. (15) and (22).

In $2H$-NbSe$_2$ the vector $\mathbf{Q} \approx \vec{a}^*/3$ is shorter than the radius of the Fermi surface centered at the Γ-point. Changes in DOS at the CDW transition for the three symmetric pairs of points *inside* the Fermi surface were directly detected in the ARPES experiment [19]. (Actually, in [19] the map of all the spots paired with the Q-vector was obtained for the whole BZ; the pattern has the hexagonal symmetry).

Recall now that theoretically the frequency of the collective excitations behaves differently at $T = T_{\mathrm{CDW}}$ for the local potentials with one or two minima [20] (see also in [18]). In the former case the frequency vanishes at the temperature of the transition. In the latter, the frequency remains finite as an ion is now "trapped" by one of the two minimum. While neutron experiments [1](b) for $2H$-TaSe$_2$ gave finite $\omega^2(Q) \approx 20$ meV^2 at $T_{\mathrm{CDW}} = 122$ K, softening of the acoustic phonons was observed for $2H$-NbSe$_2$ at $T_{\mathrm{CDW}} = 33.5$ K [14].

The difference in the phonon modes' behavior in the two materials needs a clarification. Recall that the longitudinal acoustic branch is coupled linearly with the optical mode, u of the same Σ_1- symmetry at $\mathbf{Q} = \vec{a}^*/3$. Free energy then has a contribution of the form: $F(u,s) = \omega_s^2(s^2/2) + \omega_u^2(u^2/2) + tus$, where s stands for the acoustic branch. Minimizing $F(u,s)$ and excluding u gives $F(u,s) = [\omega_s^2 - (t^2/\omega_u^2)](s^2/2)$. Let the optical mode, u be the mode that drives the transition. At $\omega_u^2(T) \to 0$ (one minimum), the acoustic mode is the first one that manifests the onset of the transition. If the potential has a few minima, the effective frequency of the acoustic mode $\omega_{s,\mathrm{eff}}^2 = [\omega_s^2 - (t^2/\omega_u^2)]$ at T_{CDW} may or may not be zero depending on the temperature behavior of $\omega_u^2(T)$. Data [1](b) for $2H$-TaSe$_2$ agree better with the second possibility.

The two $2H-$materials have different masses of Ta- and Nb- ions. It is known [20] that at lower temperatures, when quantum effects prevail, $\omega_u^2(T) \to 0$ even for a potential with a few minima. This could be another possible interpretation for the acoustic phonon frequency vanishing at $T_{\mathrm{CDW}} = 33.5$ K in the $2H$-NbSe$_2$ [14] and the finite $\omega^2(Q)$ at $T_{\mathrm{CDW}} = 122$ K in $2H$-TaSe$_2$ [1](b).

The thermodynamics of the second order phase transition would look much alike for the displacive transition [8] or for the ordering of the Ising spins. The finite $\omega^2(Q)$ at $T_{\mathrm{CDW}} = 122$ K in $2H$-TaSe$_2$ [1](b) is the first argument supporting the Ising spins model.

We argue that the temperature dependence of resistivity in all TMDC's seems to indicate in the same direction. In fact, for a broad temperature interval the resistivity, $\rho(T)$ behaves as $\rho(T) = \rho_0 + aT$, with the large intercept $\rho_0 \sim 100 - 150$ $\mu\Omega \cdot$ cm ($2H$-TaSe$_2$, [21](a, b)). This behavior is consistent with the inverse mean free time in Eq. (21) for the Green function of the form $\tau^{-1} = \tau_0^{-1} + \bar{a}T$ and $\tau_0^{-1} = (1/\pi\nu(E_F))(1 - \Lambda^{-2})$.

In the ARPES experiment [10] the self-energy, $\Sigma(\omega) = \Sigma'(\omega) + i\Sigma''(\omega)$ was measured directly on the Fermi surface of $2H$-TaSe$_2$ centered at the Γ-point of BZ. The imaginary part, $\Sigma''(\omega) \approx 60 - 70$ meV is frequency independent above T_{CDW}; this value is consistent with $\tau_0^{-1} \sim T^* = 1/\pi\nu(E_F)$. An estimate with $\tau_0^{-1} \sim T^*$ gives the right value of ρ_0 from [21](a,b).

As to the real part, $\Sigma'(\omega)$ is negligible at $T = 111$ K (i.e. above $T_{\mathrm{CDW}} = 88$ K). Below T_{CDW} $\Sigma'(\omega)$ starts to show the behavior typical for the self-energy of normal electrons interacting with phonons [7] and is peaked at the phonons frequencies ~ 50 meV. Such typical metallic signature obviously agrees with the suggestion that the CDW order parameter $g\bar{u}_i(Q)$ in Eq. (23) affects the electronic states of the energy band at the Γ-point only below the Fermi level [22, 23].

Finally, the NMR methods may help with revealing properties of the transition atoms occupying the symmetry positions in the commensurate phase of $2H$-TaSe$_2$, as it is pointed out below.

B. Quantum regime

At low T quantum effects become important in few aspects. Consider first the Schrödinger equation for an ion moving in the rigid potential $U_{\text{tot}}(u_i) = (1/\pi\nu(E_F))\bar{U}(\tilde{u}_i)$, with $\bar{U}(\tilde{u}_i)$ in the dimensionless notations. With the kinetic energy in the same notations, one has:

$$-\frac{1}{2\bar{M}}\frac{d^2}{d\tilde{u}^2}\Psi(\tilde{u}) + [\bar{U}(\tilde{u}) - \bar{E}]\Psi(\tilde{u}) = 0 \qquad (25)$$

The dimensionless "mass", $\bar{M}$ in (25) is defined by $1/\bar{M} = [\pi\nu(E_F)\omega_0]^2/2$. (The adiabatic parameter $1/\sqrt{\bar{M}} = (\pi\nu(E_F)\omega_0)/\sqrt{2}$ is about one tenth in $2H$-NbSe$_2$).

For the single-minimum well ($\Lambda^2 < 1$) quantum effects are important when $T_{CDW} < \omega_0$. The lattice oscillations are now quantized and the electronic Green function is "dressed" by phonons. In the adiabatic approximations, solution for the problem of interacting electrons and phonons in normal metals was given many years ago in [7].

At first glance, Eq. (25) adds a possibility of quantum tunneling between minima of the two-well potential [20]. Actually, Eq. (25) could account only for tunneling in a "rigid" potential, a potential built in the lattice only by the inter-atomic forces. The two-well potential (Eqs. (9,15)) is formed by interactions between electrons and the local lattice distortions. It was emphasized in [11] in connection with the martensitic transitions in Nb$_3$Sn and V$_3$Si, that at the tunneling event, at which the ion goes over, say, from u_+ to u_-, the electronic configuration reverses as well. Such a feature cannot be described in terms of Eq. (25). According to [11], the under-barrier tunneling results in a Kondo-like quantum regime at which the height of the barrier would diminish with temperature. The parameter $\sqrt{\bar{M}}$ stands in the exponent of the expression for the tunneling matrix element. With no closed solution found in [11] one may only argue that with the value of $\sqrt{\bar{M}} \sim 10$ the Kondo-like regime [11] is probably of no relevance to the CDW physics in TMDC.

Below the transition in the CDW ground state ions will occupy their proper minima, in accordance with the superlattice pattern [1](b) and tunneling between minima must stop. Nevertheless, experimentally, the pattern reveals an interesting peculiarity. Indeed, in the CDW phase one in three atoms along the symmetry lines finds itself in the position with the trigonal symmetry ($2H$-TaSe$_2$ [1](b); see Fig. 4 in [12]). While below transition the intersite interactions do indeed arrest quantum tunneling between minima for the other two of the three atoms, the degeneracy is not lifted for the atom in this symmetric position.

NMR experiments seem be able to verify the very concept of the two minima-potential by studying the ions in positions with the trigonal symmetry.

According to ARPES data [9], the CDW transition in $2H$-NbSe$_2$ slightly affects only the two-barrel Fermi surface at the K-point in BZ, while FS at the Γ-point remains intact. The three Q-vectors couple together the three points on the inner FS at K, which are seen experimentally with small but observable gaps at these points. Surprisingly, the observation of such small local gaps (~ 2.4 meV) was interpreted in [9] as the conclusive proof in favor of the nesting mechanism of the CDW formation.

The physics of strong local e-ph interaction bring us back to the Holstein model [16] of electrons interacting with dispersionless phonons. No exact solution is known for the Holstein model either, but its low temperature physics was investigated numerically in DMFT (Dynamical Mean Field Theory, [24]) approximation. (For a brief summary of results for the Holstein model at $T = 0$ see [25]).

The DMFT approach is strictly local. Intersite interactions (see Eq. (18)) and the CDW transition itself cannot be treated by DMFT. Here we indicate parallels between our physics above and the results [25] at $T = 0$ for the Holstein model. Among them are: (1) The double-well potential that develops when the e-ph coupling constant becomes larger some critical value; (2) Large imaginary part in the Green function: Spectral Function extends over the energy interval that significantly exceeds the phonon frequency (compare with our Eq. (22)); (3) The ground state remains metallic (at least for not-too-strong e-ph coupling).

In [25] the mass of electronic excitations increases as the residue at the pole of the electronic Green function decreases.

Judging by these results, the physics studied above allows its extension into the low temperature regime.

V. SUMMARY

In summary, we calculated the local elastic energy for single ion by re-summing exactly the electron-lattice interactions in the real space. Strong *e-ph* interactions qualitatively change the local environment by binding ions and electrons together, thus breaking the adiabatic approximation. The concept is the realization of the Migdal instability different from that one considered in [8]. The CDW transition takes the form of a phase transition in the system of interacting Ising spins. The value of the structural vector **Q** and parameters of the Fermi surfaces being not related with each other, the energy spectrum of electrons remains metallic below the temperature of the CDW transition. The CDW gap seen in the tunneling experiments below the transition is defined in terms of reduced DOS inside the electronic bands. Its large value is consistent with the energies of the deep minima of the local potential. Other experimental evidences in favor of the Ising model were enumerated. The electronic properties of the transition-metal dichalcogenides, as they are seen by ARPES, agree well with the suggested concept.

Conclusions from the analytical results derived in the classical regime can be extended to lower temperatures as it follows from the comparison with numerical results for the Holstein model.

VI. ACKNOWLEDGMENTS

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