

Breakdown of the Migdal-Eliashberg theory in the strong-coupling adiabatic regime

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In view of some recent works on the role of vertex corrections in the electron-phonon system we readdress an important question of the validity of the Migdal-Eliashberg theory. Based on the solution of the Holstein model and $1/\lambda$ strong-coupling expansion, we argue that the standard Feynman-Dyson perturbation theory by Migdal and Eliashberg *with* or *without* vertex corrections cannot be applied if the electron-phonon coupling is strong ($\lambda \geq 1$) at any ratio of the phonon, ω and Fermi, E_F energies. In the extreme adiabatic limit ($\omega \ll E_F$) of the Holstein model electrons collapse into self-trapped small polarons or bipolarons due to spontaneous translational-symmetry breaking at $\lambda \simeq 1$. With the increasing phonon frequency the region of the applicability of the theory shrinks to lower values of $\lambda < 1$.

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The theory of ordinary metals is based on 'Migdal's' theorem [1], which showed that the contribution of the diagrams with 'crossing' phonon lines (so called 'vertex' corrections) is small. This is true if the parameter $\lambda\omega/E_F$ is small. Neglecting the vertex corrections Migdal calculated the renormalised electron mass as $m^* = m(1 + \lambda)$ (near the Fermi level) [1] and by breaking the gauge symmetry Eliashberg extended the Migdal theory to describe the BCS superconducting state at intermediate values of λ [2]. The same theory, applied to phonons, yields the renormalised phonon frequency $\tilde{\omega} = \omega(1 - 2\lambda)^{1/2}$ [1] with an instability at $\lambda = 0.5$. Because of this instability both Migdal [1] and Eliashberg [2] restricted the applicability of their approach to $\lambda \leq 1$.

It was then shown that if the adiabatic Born-Oppenheimer approach is properly applied to a metal, there is only negligible renormalisation of the phonon frequencies of the order of the adiabatic ratio, $\omega/E_F \ll 1$ for *any* value of λ [3]. The conclusion was that the standard electron-phonon interaction could be applied to electrons for any value of λ but it should not be applied to renormalise phonons [4]. As a result, many authors used the Migdal-Eliashberg theory with λ much larger than 1 (see, for example, Ref. [5]).

However, starting from the infinite coupling limit, $\lambda = \infty$ and applying the inverse ($1/\lambda$) expansion technique [6] we showed [7–9] that the many-electron system collapses into small polaron regime at $\lambda \sim 1$ almost independent of the adiabatic ratio. This regime is beyond the Migdal-Eliashberg theory. It cannot be reached by summation of the standard Feynman-Dyson perturbation diagrams even including *all* vertex corrections, because of the broken translational symmetry, as first discussed by Landau

[10] for a single electron and by us [8] for the many-electron system. During last years quite a few numerical and analytical studies have confirmed this conclusion [11–28] (and references therein). On the other hand a few others (see, for example, [29,30]) still argue that the breakdown of the Migdal-Eliashberg theory might happen only at $\lambda \geq E_F/\omega \gg 1$. Indeed numerical study of the finite bandwidth effects [31] and some analytical calculations of the vertex corrections to the vertex function [32,33,30] with the standard Feynman-Dyson perturbation technique confirm the second conclusion.

In this letter I compare the Migdal solution of the Holstein Hamiltonian with the exact one in the extreme adiabatic regime, $\omega/E_F \rightarrow 0$, to show that the ground state of the system is a self-trapped insulating state with broken translational symmetry already at $\lambda \geq 1$.

The vertex corrections and the finite bandwidth are rather technical issues, playing no role in the extreme adiabatic limit [1,32,31]. There is, however, another basic assumption of the canonical Migdal-Eliashberg theory. That is the electron and phonon Green functions (GF) are translationally invariant. As a result one takes $G(\mathbf{r}, \mathbf{r}', \tau) = G(\mathbf{r} - \mathbf{r}', \tau)$ with Fourier component $G(\mathbf{k}, \Omega)$ prior to solving the Dyson equations. This assumption excludes the possibility of local violation of the translational symmetry due to the lattice deformation in any order of the Feynman-Dyson perturbation theory. This is similar to the absence of the anomalous (Bogoliubov) averages in any order of the perturbation theory. To enable electrons to relax into the lowest polaronic states, one has to introduce an infinitesimal translationally non-invariant potential, which should be set equal to zero only in the final solution for the GF [8]. As in the case of the off-diagonal superconducting order parameter, a small translational-symmetry-breaking potential drives the system into a new ground state at sufficiently large coupling, $\lambda \sim 1$, independent of the adiabatic ratio. Setting it equal to zero in the solution of the equations of motion restores the translational symmetry but in a new polaronic band rather than in the bare electron band, which turns out to be an excited state.

In particular, let us consider the extreme adiabatic limit of the Holstein chain [34], which has the simple analytical solution:

$$H = -t \sum_{\langle ij \rangle} c_i^\dagger c_j + H.c. + 2(\lambda kt)^{1/2} \sum_i x_i c_i^\dagger c_i + \sum_i \left(-\frac{1}{2M} \frac{\partial^2}{\partial x_i^2} + \frac{kx_i^2}{2} \right), \quad (1)$$

where t is the nearest neighbour hopping integral, c_i^\dagger, c_i are the electron operators, x_i is the normal coordinate of the molecule (site) i , and $k = M\omega$ with M the ion mass [35]. We first consider the two-site case (zero dimensional limit), $i, j = 1, 2$ with one electron, and then generalise the result for the infinite lattice with many electrons. The transformation $X = (x_1 + x_2)$, $\xi = x_1 - x_2$ allows us to eliminate the coordinate X , which is coupled only with the total density ($n_1 + n_2 = 1$), leaving the following Hamiltonian to solve in the extreme adiabatic limit $M \rightarrow \infty$:

$$H = -t(c_1^\dagger c_2 + c_2^\dagger c_1) + (\lambda kt)^{1/2} \xi (c_1^\dagger c_1 - c_2^\dagger c_2) + \frac{k\xi^2}{4}. \quad (2)$$

The solution is

$$\psi = (\alpha c_1^\dagger + \beta c_2^\dagger) |0\rangle, \quad (3)$$

where

$$\alpha = \frac{t}{[t^2 + ((\lambda kt)^{1/2} \xi + (t^2 + \lambda kt \xi^2)^{1/2})^2]^{1/2}}, \quad (4)$$

$$\beta = -\frac{(\lambda kt)^{1/2} \xi + (t^2 + \lambda kt \xi^2)^{1/2}}{[t^2 + ((\lambda kt)^{1/2} \xi + (t^2 + \lambda kt \xi^2)^{1/2})^2]^{1/2}}, \quad (5)$$

and the energy

$$E = \frac{k\xi^2}{4} - (t^2 + \lambda kt \xi^2)^{1/2}. \quad (6)$$

In the extreme adiabatic limit the displacement ξ is classical, so the ground state energy, E_0 and the ground state displacement ξ_0 are obtained by minimising Eq.(6) with respect to ξ . If $\lambda \geq 0.5$ one obtains

$$E_0 = -t\left(\lambda + \frac{1}{4\lambda}\right), \quad (7)$$

and

$$\xi_0 = \left[\frac{t(4\lambda^2 - 1)}{\lambda k} \right]^{1/2}. \quad (8)$$

The symmetry-breaking ('order') parameter is

$$\Delta \equiv \beta^2 - \alpha^2 = \frac{[2\lambda + (4\lambda^2 - 1)^{1/2}]^2 - 1}{[2\lambda + (4\lambda^2 - 1)^{1/2}]^2 + 1}. \quad (9)$$

If, however, $\lambda < 0.5$ the ground state is translationally invariant with $E_0 = -t, \xi = 0, \beta = -\alpha$, and $\Delta = 0$. Precisely this state is the 'Migdal' solution of the Holstein model. Indeed, in the Migdal approximation GF is diagonal in the \mathbf{k} representation, $G(\mathbf{k}, \mathbf{k}', \tau) = G(\mathbf{k}, \tau) \delta_{\mathbf{k}, \mathbf{k}'}$. The site operators can be transformed into momentum space as

$$c_k = N^{-1/2} \sum_j c_j \exp(ika_j), \quad (10)$$

with a the lattice constant, N the number of sites, and $k = 2\pi n/Na$ with $-N/2 < n \leq N/2$. Then the off-diagonal GF with $k = 0$ and $k' = \pi/a$ of the two-site chain ($N = 2$) at $\tau = -0$ is given by

$$G(k, k', -0) = \frac{i}{2} \langle (c_1^\dagger - c_2^\dagger)(c_1 + c_2) \rangle. \quad (11)$$

Calculating this average one obtains

$$G(k, k', -0) = \frac{i}{2} (\alpha^2 - \beta^2), \quad (12)$$

which should vanish in the Migdal theory. Hence, this theory only provides symmetric (translationally invariant) solution with $|\alpha| = |\beta|$. When $\lambda > 0.5$ this solution is *not* the ground state of the system, Fig.1. The system collapses into a localised adiabatic polaron, trapped on the 'right' (or on the 'left') site due to a finite local lattice deformation ξ_0 . On the other hand, when $\lambda < 0.5$, the Migdal solution is the *only* solution with $\xi_0 = 0$. Thus the Migdal-Eliashberg constraint [1,2] on the applicability of their approach is perfectly correct irrespective of the phonon frequency renormalisation.

The generalisation to the multi-polaron system on the infinite lattice of any dimension is straightforward in the extreme adiabatic regime. The adiabatic solution of the infinite one-dimensional (1D) chain with one electron was obtained by Rashba [36] in the continuous approximation, and by Holstein [34] and Kabanov and Mashtakov [11] for a discrete lattice. The last authors also studied the Holstein two-dimensional (2D) and three-dimensional (3D) lattices in the adiabatic limit. According to Ref. [11] the self-trapping of a single electron occurs for any value of λ in a 1D Holstein chain, and at $\lambda \geq 0.875$ and $\lambda \geq 0.92$ in 2D and 3D, respectively. The single-polaron GF is not translationally invariant in this strong-coupling adiabatic limit. The radius of the self-trapped adiabatic polaron, r_p , is readily derived from its continuous wave function [36]

$$\psi(x) \sim 1/\cosh(\lambda x/a). \quad (13)$$

It becomes smaller than the lattice constant, $r_p = a/\lambda$ for $\lambda \geq 1$. That is why in the strong-coupling ($\lambda \geq 1$) adiabatic regime the multi-polaron system remains in the self-trapped insulating state no matter how many polarons it has. The only instability which might occur in this regime is the formation of on-site self-trapped bipolarons, if the Holstein on-site attractive interaction, $2\lambda zt$, is larger than the repulsive Hubbard U [37]. Actually, this instability can be seen in the second order Feynman-Dyson diagram containing the polarisation loop, as explained in Ref. [38]. On-site bipolarons form a charge ordered insulating state due to weak repulsion between

them [39]. The exact analytical and numerical proof of this statement as well as different polaronic and bipolaronic configurations in the adiabatic Holstein model was reviewed by Aubry [40]. For example, the asymptotically exact many-particle ground state of the half-filled Holstein model in the strong-coupling limit ($\lambda \gg 1$) is

$$\psi = \prod_{j \in B} c_{j,\uparrow}^\dagger c_{j,\downarrow}^\dagger |0\rangle \quad (14)$$

for any value of the adiabatic ratio, ω/zt [39,40]. Here j are B -sites of the bipartite lattice $A + B$. It is a charged ordered insulating state, rather than the Fermi liquid, expected in the Migdal approximation at any value of λ in the extreme adiabatic limit, $\omega \rightarrow 0$. If the Coulomb repulsion (Hubbard U) is sufficiently strong to prevent the bipolaron formation, than at half filling every site is occupied by one polaron. The deformation barrier for their tunneling to a neighboring site disappears, so one could erroneously believe that the system should be metallic. However, to keep polarons unbound into on-site bipolarons, the Hubbard U should be larger than $2\lambda zt$, i.e. larger than the bandwidth, $U > 2zt$, if $\lambda > 1$. It is well known that in this regime the system is a Mott-Hubbard insulator, rather than an ordinary metal. Hence, the Migdal-Eliashberg theory cannot be applied at $\lambda \geq 1$, no matter what a strength of the Coulomb interaction, the number of electrons and the dimension of the lattice are.

The non-adiabatic corrections (phonons) allow polarons and bipolarons propagate as Bloch waves in a new (narrow) band. Thus, under certain conditions [28] the multipolaron system might be metallic with polaronic (or bipolaronic) carriers rather than bare electrons. However, there is a qualitative difference between the ordinary Fermi liquid and the polaronic one. In particular, the renormalized (effective) mass of electrons is independent of the ion mass M in ordinary metals (where the Migdal adiabatic approximation is believed to be valid), because λ does not depend on the isotope mass. However, the polaron effective mass m^* will depend on M . This is because the polaron mass $m^* = m \exp(A/\omega)$ [41], where m is the band mass in the absence of the electron-phonon interaction, and A is a constant. Hence, there is a large isotope effect on the carrier mass in polaronic metals, in contrast to the zero isotope effect in ordinary metals. Recently, this effect has been experimentally found in cuprates [42] and manganites [43]. With the increasing phonon frequency the $1/\lambda$ polaron expansion becomes valid for a smaller values of λ (see, for example, [28]). Hence, the region of the applicability of the Migdal approach shrinks with increasing ω to the smaller values of the coupling, $\lambda < 1$.

The essential physics of strongly coupled electrons and phonons has been understood with the $1/\lambda$ expansion technique [9,16], which starts with the exact solution in the extreme limit $\lambda = \infty$ and allows for the summation

of all multiphonon diagrams in any order of the small parameter $1/\lambda$ for any value of the adiabatic ratio ω/t . It predicts a breakdown of the Migdal-Eliashberg theory at $\lambda \simeq 1$ or less, in agreement with the exact solution of the extreme adiabatic Holstein model discussed here. There are also other studies of the same problem, which do not rely on the standard Feynman-Dyson perturbation theory in powers of λ . In particular, Takada *et al* [17,20,44] applied the gauge-invariant self-consistent method neglecting the vector term in the Ward identity. Benedetti and Zeyher [23] applied the dynamical mean-field theory in infinite dimensions. As in the $1/\lambda$ expansion technique, both approaches avoided the problem of the broken translational symmetry by using the nondispersive vertex and Green functions as the starting point. As a result they arrived at the same correct conclusion about the applicability of the Migdal approach (in Ref. [23] the critical value of λ was found to be 1.3 in the adiabatic limit). Meanwhile, some authors [30,29], who rely on the perturbation expansion in powers of λ , fail to notice the self-trapping transition, erroneously claiming that the Migdal-Eliashberg theory could be applied at practically any λ in the extreme adiabatic regime.

In conclusion, I have shown that the Migdal-Eliashberg theory cannot be applied in the adiabatic regime of the strongly coupled many-electron system if the (BCS) coupling constant, λ , is about 1 or larger irrespective of the number of electrons. There is a transition into the self-trapped state due to the broken translational symmetry, Fig.1. The transition appears at $0.5 < \lambda < 1.3$ depending on the lattice dimensionality. Naturally, with the increasing phonon frequency the region of the applicability of the Migdal approach shrinks further to lower values of λ . I believe that this conclusion is correct for any electron-phonon interaction conserving the on-site electron occupation numbers. In particular, Hiramoto and Toyozawa [45] calculated the strength of the deformation potential, which transforms electrons into small polarons and bipolarons. Their continuous approach is sufficient for a qualitative estimate if the Debye wavenumber $q_D \sim \pi/a$ is introduced as an upper limit cut-off in all sums in the momentum space. Hiramoto and Toyozawa found that the transition between two electrons and a small bipolaron occurs at $\lambda \simeq 0.5$, that is half of the critical value of λ at which the transition from electron to small polaron takes place in the extreme adiabatic limit ($sq_D \ll zt$, s the sound velocity). The effect of the adiabatic ratio sq_D/zt on the critical value of λ was found to be negligible. The radius of the acoustic polaron and bipolaron is the lattice constant, so the critical λ does not depend on the number of electrons in this case either.

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Figure caption

Fig.1. The ground state energy (solid line), E/t , and the 'order' parameter (thin line), Δ , of the adiabatic Holstein model as functions of the coupling constant, λ . There is the symmetry breaking transition at $\lambda = 0.5$. The energy of the symmetric state is shown by the dashed line.

