Supplemental Material to the article

"Light quark masses in a theory with dynamical chiral symmetry breaking"

To obtain a meson Lagrangian from the four-quark interactions of Nambu–Jona-Lasinio (NJL) type, one should isolate the divergent part of the one-loop quark diagrams, which dominate the low-energy regime of the effective theory. The proper-time Fock–Schwinger method is known to be an efficient tool for this purpose. However, the direct use of this method is problematic if the quark masses are not equal. Till recently, the isolation of the singular part of one-loop quark diagrams in the NJL model was carried out due to one or another ansatz superimposed on the form of regularized integrals. Such a procedure is ambiguous, since it is always possible to propose another ansatz that differs by adding to the considered integral an arbitrary finite contribution that vanishes in the limit of equal quark masses. To define such a procedure unambiguously, a mathematically rigorous method is required. The Volterra series combined with the Fock–Schwinger proper-time method allows to solve the problem.

A Volterra representation generalizes the standard large mass expansion of the heat kernel to the case of unequal masses by the formula

$$e^{-t(M^2+A)} = e^{-tM^2}\left[1+\sum_{n=1}^{\infty}(-1)^n f_n(t,A)\right], \tag{1}$$

where $M=\mathrm{diag}(M_u,M_d,M_s)$ is a diagonal mass matrix; t is the Fock–Schwinger proper-time parameter; the expression in the square brackets is the time-ordered exponential $\mathrm{OE}[-A](t)$ of $A(s)=e^{sM^2}A\,e^{-sM^2}$, and A is a positive definite self-adjoint elliptic operator in some background. The coefficients of the series (1) are

$$f_n(t,A)=\int_0^t ds_1\int_0^{s_1} ds_2\ldots\int_0^{s_{n-1}} ds_n A(s_1)A(s_2)\ldots A(s_n). \tag{2}$$

In the case of equal masses $M_u=M_d=M_s$, this formula yields the well-known large mass expansion with standard Seeley–DeWitt coefficients $a_n(x,y)$. If the masses are not equal, formula (1) can be thought of as a natural extension of the Schwinger's method used to isolate the divergent aspects of a calculation in integrals with respect to the proper-time to the non-commutative algebra. Unlike the commutative case, the products (2) are spread over a certain time interval, and the reason is the unequal quark masses.

To exclude quark degrees of freedom in the Lagrangian density

$$\mathcal{L}_{\mathrm{QQ}}=\bar{Q}(i\gamma^\mu d_\mu - M+\sigma)Q=\bar{Q}DQ, \tag{3}$$

one should integrate over quark variables in the corresponding functional integral. The result is a functional determinant

$$W_E=\ln|\det D_E| = -\int_0^\infty \frac{dt}{2t}\,\rho_{t,\Lambda}\,\mathrm{Tr}\left(e^{-tD_E^\dagger D_E}\right), \tag{4}$$

representing a real part of the one-loop effective action in Euclidian space as the integral over the proper-time t.

The functional trace in (4) can be evaluated by the Schwinger technique of a fictitious Hilbert space. The use of a plane wave with Euclidian 4-momenta k, $\langle x|k\rangle$, as a basis greatly simplifies the calculations (details are given in [8]) and leads to the representation of the functional trace by the integrals over coordinates and momenta

$$W_E=-\int d^4x\int\frac{d^4k}{(2\pi)^4}\,e^{-k^2}\int_0^\infty\frac{dt}{2t^3}\,\rho_{t,\Lambda}\,\mathrm{tr}_I\left[e^{-t(M^2+A)}\right], \tag{5}$$

where we use the proper-time regularization $\rho_{t,\Lambda}$ with two subtractions at scale Λ

$$\rho_{t,\Lambda} = 1 - (1 + t\Lambda^2)e^{-t\Lambda^2}. \tag{6}$$

It totally agrees with the regularization of the standard NJL model [14]. A self-adjoint operator in Hilbert space A is

$$A = -d^2 - 2ikd/\sqrt{t} + Y, \tag{7}$$

where a summation over four-vector indices is implicit. The covariant derivative

$$d_\alpha = \partial_\alpha + i\Gamma_\alpha, \tag{8}$$
$$\Gamma_\alpha = V_\alpha - \xi_\alpha^{(+)} + \gamma_5(A_\alpha - \xi_\alpha^{(-)}), \tag{9}$$

where Γ_α is a connection in a curved factor space of Goldstone fields, and

$$\begin{aligned} Y = & \,\sigma^2 - \{\sigma, M\} + i[\gamma_\alpha(\sigma - M), d_\alpha] \\ & + \frac{1}{4}[\gamma_\alpha, \gamma_\beta][d_\alpha, d_\beta]. \end{aligned} \tag{10}$$

Inserting Eq. (1) into (5) with the following integrations over four-momenta k_α and the proper-time t one finds the one-quark-loop (1QL) contribution to the effective meson Lagrangian in the form of asymptotic series

$$\mathcal{L}_{\rm 1QL} = -\frac{N_c}{32\pi^2} \sum_{n=1}^{\infty} \mathrm{tr}\, b_n(x,x), \tag{11}$$

where coefficients $b_n(x,x)$ depend on the external fields and quark masses. They contain a full information about both the effective meson vertices and corresponding coupling constants. The first two coefficients are [8]

$$\mathrm{tr}\, b_1 = \mathrm{tr}_{Df} \left[-J_0 \circ Y - \frac{1}{4}(\Delta J_0 \circ \Gamma_\mu)\Gamma^\mu \right], \tag{12}$$

$$\begin{aligned} \mathrm{tr}\, b_2 = & \,\frac{1}{2}\mathrm{tr}_{Df} \left[Y(J \circ Y) - \frac{1}{6}\Gamma^{\mu\nu}(J \circ \Gamma_{\mu\nu}) \right] \\ & + \mathrm{tr}_D\, \Delta b_2. \end{aligned} \tag{13}$$

The traces are taken over Dirac (D) gamma matrices and flavor (f) indices. Other notations correspond to [8].

Let us explain what is the difference between formulas (12) and (13) from the expressions of the standard NJL model. There are several. The standard NJL Lagrangian contains only divergent parts of one-loop quark diagrams. In our formulas, they correspond to the first term in (12) and the first two terms in (13). If the masses of the quarks were equal, these terms would completely coincide with the Lagrangian of the standard NJL model (in the same limiting case). In other words, both Lagrangians are equivalent in the chiral limit. In the case of unequal quark masses, the theories differ substantially. This concerns both the terms already considered and the set of additional vertices contained in the second term in (12) and the third term in (13). The peculiarity of the latter is that they are finite and vanish in the chiral limit. These terms break both isotopic and $SU(3)_f$ symmetry. However, it is not yet clear their physical role. Our longstanding goal is to elucidate the physical content of this new theory.

Thus, the effective meson Lagrangian is given by

$$\begin{aligned} \mathcal{L}_{\rm eff} = & \,\mathcal{L}_{\rm 1QL} + \frac{1}{4G_V}\mathrm{tr}\,(V_\mu^2 + A_\mu^2) \\ & - \frac{1}{4G_S}\mathrm{tr}\,\left[\sigma^2 - \{\sigma, M\} + (\sigma - M)\Sigma\right]. \end{aligned} \tag{14}$$

This Lagrangian contains all the information about chiral symmetry breaking, including effects induced by unequal quark masses. In what follows we will be interested only in the part of this Lagrangian that is responsible for the physics of pseudoscalar mesons.

First of all, it is necessary to exclude from this Lagrangian the contribution of terms linear in the scalar field. It is contained in $\mathcal{L}_{1\mathrm{QL}}$ and the last term in (14). Noticing that

$$\mathrm{tr}_{Df}\left(-J_0 \circ Y\right) \to 8 \sum_{i=u,d,s} J_0(M_i) M_i \sigma_i, \tag{15}$$

we arrive at the self-consistency equation relating the masses of light quarks m_i to the masses of heavy constituent quarks M_i

$$M_i \left(1 - \frac{N_c G_S}{2\pi^2} J_0(M_i)\right) = m_i. \tag{16}$$

To pass to physical fields, it is necessary to eliminate the mixing of pseudoscalar fields with axial-vector ones (PA-mixing), and also to separate the kinetic part of the free Lagrangian of pseudoscalars in $\mathcal{L}_{1\mathrm{QL}}$.

The first goal is achieved by redefining the axial vector field $A_\mu = A'_\mu - \kappa_A \circ \xi^{(-)}_\mu$. In this case the corresponding contributions from $\mathcal{L}_{1\mathrm{QL}}$ and the second term in (14) can be canceled. To demonstrate this, collect the necessary terms of the effective Lagrangian

$$\begin{aligned}
\mathcal{L}^{(b_1)}_{1\mathrm{QL}} \to \frac{N_c}{32\pi^2} \Big\{ & (\Delta J_0)_{ud} \left[(1-\kappa_{Aud})\partial_\mu \pi^+ + 2a'^{+}_{1\mu}\right] \\
\times & \left[(1-\kappa_{Aud})\partial_\mu \pi^- + 2a'^{-}_{1\mu}\right] \\
+ & (\Delta J_0)_{us} \left[(1-\kappa_{Aus})\partial_\mu K^+ + 2K'^{+}_{1A\mu}\right] \\
\times & \left[(1-\kappa_{Aus})\partial_\mu K^- + 2K'^{-}_{1A\mu}\right] \\
+ & (\Delta J_0)_{ds} \left[(1-\kappa_{Ads})\partial_\mu K^0 + 2K'^{0}_{1A\mu}\right] \\
\times & \left[(1-\kappa_{Ads})\partial_\mu \bar{K}^0 + 2\bar{K}'^{0}_{1A\mu}\right] \Big\},
\end{aligned} \tag{17}$$

where the symbol (b_1) indicates the origin of the contribution in question. Recall that one-loop factors $(\Delta J_0)_{ij}$ are finite and vanish in the limit of equal quark masses. There are no such contributions in the standard version of the NJL model.

The next contribution owes its origin to the coefficient b_2, namely its part described by the first term of Eq. (13)

$$\begin{aligned}
\mathcal{L}^{(b_2)}_{1\mathrm{QL}} \to & \frac{N_c}{16\pi^2} \Big\{ (M_u + M_d)^2 J_1(M_u, M_d) \\
\times & \left[(1-\kappa_{Aud})\partial_\mu \pi^+ + 2a'^{+}_{1\mu}\right] \left[(1-\kappa_{Aud})\partial_\mu \pi^- + 2a'^{-}_{1\mu}\right] \\
+ & (M_u + M_s)^2 J_1(M_u, M_s) \left[(1-\kappa_{Aus})\partial_\mu K^+ + 2K'^{+}_{1A\mu}\right] \\
\times & \left[(1-\kappa_{Aus})\partial_\mu K^- + 2K'^{-}_{1A\mu}\right] \\
+ & (M_d + M_s)^2 J_1(M_d, M_s) \left[(1-\kappa_{Ads})\partial_\mu K^0 + 2K'^{0}_{1A\mu}\right] \\
\times & \left[(1-\kappa_{Ads})\partial_\mu \bar{K}^0 + 2\bar{K}'^{0}_{1A\mu}\right] \Big\}.
\end{aligned} \tag{18}$$

Here, the regularized logarithmically divergent integral $J_1(M_i, M_j)$ coincides up to a common factor with the corresponding one-loop integral $I_2(M_i, M_j)$ used in the standard approach (see Eq. (13) in [14]). We emphasize that the regularization used by us was deliberately chosen in such a way as to be totally consistent with the standard approach.

It remains to take into account the last contribution related to the PA-mixing, which arises from the second term in (14). This contribution is

$$\begin{aligned}
-\frac{1}{2G_V} \Big(& \kappa_{Aud} a'^{-}_{1\mu} \partial_\mu \pi^+ + \kappa_{Aus} K'^{-}_{1A\mu} \partial_\mu K^+ \\
& + \kappa_{Ads} \bar{K}'^{0}_{1A\mu} \partial_\mu K^0 \Big) + \mathrm{h.c.}
\end{aligned} \tag{19}$$

Collecting the results (17), (18) and (19), we find

$$\kappa_{Aij}^{-1} = 1 + \frac{8\pi^2}{N_c G_V [2(M_i + M_j)^2 J_{1ij} + \Delta J_{0ij}]}. \tag{20}$$

What is new here is the appearance of the term ΔJ_{0ij}, which is absent in the standard picture. It is the contributions of such finite terms (as it has been shown in [8] there are over a hundred of them in the effective Lagrangian (14)), which vanish in the limit of equal quark masses, that could not be taken into account in the standard approach. The method considered here makes it possible to do this systematically. As a result, an interesting opportunity arises to study their role in the complex process of dynamic and explicit chiral symmetry breaking. Of course, any effective theory (for example, $1/N_c$ chiral perturbation theory [3]) takes into account these effects, but at the cost of a large number of arbitrary constants. In a theory with four-quark interactions, the inclusion of such terms does not require the introducing of new parameters, thereby allowing one to calculate the constants of the effective chiral Lagrangian.

Our next task is to obtain the kinetic part of the free Lagrangian of pseudoscalar fields. To do this, we need the already known expressions (17), (18) and, in addition, one should write out the corresponding contribution of the second term in (14), that was omitted in (19)

$$\begin{aligned} &\frac{1}{4G_V}\left(\kappa_{Aud}^2 \partial_\mu \pi^+ \partial_\mu \pi^- + \kappa_{Aus}^2 \partial_\mu K^+ \partial_\mu K^- \right. \\ &\qquad \left. + \kappa_{Ads}^2 \partial_\mu \bar{K}^0 \partial_\mu K^0 \right). \end{aligned} \tag{21}$$

Collecting all these contributions, one finds, for instance in the case of charged pions, that kinetic term is given by

$$\begin{aligned} \mathcal{L}_{\text{kin}}^{\pi^+\pi^-} &= \partial_\mu \pi^+ \partial_\mu \pi^- \left\{ \frac{\kappa_{Aud}^2}{4G_V} + \frac{N_c}{32\pi^2}(1-\kappa_{Aud})^2 \right. \\ &\times \left. [2(M_u + M_d)^2 J_1(M_u, M_d) + \Delta J_{0ud}] \right\} \\ &= \left(\frac{\kappa_{Aud}}{4G_V}\right) \partial_\mu \pi^+ \partial_\mu \pi^- . \end{aligned} \tag{22}$$

To give this expression a standard form, one should introduce the physical pion fields π_{ph}

$$\pi = \sqrt{\frac{4G_V}{\kappa_{Aud}}}\, \pi^{\text{ph}} = \frac{1}{f_\pi}\, \pi_{\text{ph}}. \tag{23}$$

The dimensional parameter f_π is nothing else than the weak decay constant of a charged pion. Similar calculations in the case of kaons give the values of the constants

$$f_{K^+} = \sqrt{\frac{\kappa_{Aus}}{4G_V}}, \quad f_{K^0} = \sqrt{\frac{\kappa_{Ads}}{4G_V}}. \tag{24}$$

The resulting expressions require a more detailed discussion. First, they differ from the standard result of the NJL model, where the constant f_π is estimated through the Goldberger–Treiman relation on the quark level. The latter is a result of current algebra. It can be easily shown that in the chiral limit the formula (23) coincides with the result of the standard approach. Second, the behavior of the constants beyond chiral limit is essentially different. The absence of a clear procedure for taking into account the effects of explicit chiral symmetry breaking in the standard approach makes it impossible, for instance, to obtain the experimental value of the ratio $f_K/f_\pi = 1.19$. On the contrary, the method proposed in our work, as we saw in the main text of the article, easily copes with this task and leads to a phenomenologically consistent value $f_K/f_\pi = 1.21$. This agreement is achieved due to the additional contribution from $(\Delta J_0)_{us}$ term.

Let's establish now the mass formulas of $\pi^\pm$, $K^\pm$, K^0 and $\bar{K}^0$ mesons. To do this, we need the corresponding contribution arising from the last term of the Lagrangian (14)

$$
\begin{aligned}
\frac{1}{4G_S}\mathrm{tr}_f\, M\Sigma \to\ & -\frac{1}{4G_S}\big[(M_u+M_d)(m_u+m_d)\pi^+\pi^- \\
& + (M_u+M_s)(m_u+m_s)K^+K^- \\
& + (M_d+M_s)(m_d+m_s)\bar{K}^0K^0\big]\,. \qquad (25)
\end{aligned}
$$

Note that integration over quark fields, i.e., the Lagrangian $\mathcal{L}_{\rm 1QL}$, does not contribute to the pseudoscalar masses.

Now, after redefinitions of fields, we finally arrive to the result

$$
\begin{aligned}
\mathcal{L}_{\rm mass} = & -\frac{G_V}{G_S}\left[\frac{1}{\kappa_{Aud}}(M_u+M_d)(m_u+m_d)\pi^+_{\rm ph}\pi^-_{\rm ph}\right. \\
& + \frac{1}{\kappa_{Aus}}(M_u+M_s)(m_u+m_s)K^+_{\rm ph}K^-_{\rm ph} \\
& + \left.\frac{1}{\kappa_{Ads}}(M_d+M_s)(m_d+m_s)\bar{K}^0_{\rm ph}K^0_{\rm ph}\right]. \qquad (26)
\end{aligned}
$$

Expanding these expressions in powers of light quarks, one can not only obtain the known result of the current algebra: $\bar{\mu}^2_{\pi^\pm} = B_0(m_u+m_d)$, $\bar{\mu}^2_{K^\pm} = B_0(m_u+m_s)$ and $\bar{\mu}^2_{K^0} = B_0(m_d+m_s)$, but also move further by calculating the corrections to the current algebra mass formulae, as it was demonstrated in the main text of the article.