

Fermion correlation function in multiple field configurations

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A simple quantum-mechanical example is used to analyze the effect of field configuration copying on a fermion correlation function. It is shown that the copying procedure may result in a large correction to the fermion effective mass except for short-time correlations in the low-temperature regime. This correction possibly explains the oscillatory behavior of meson effective masses in a recent lattice QCD calculation.

Since the early 1980s lattice theorists have frequently applied the following technique: time size of a lattice is artificially enlarged by copying gauge configurations several times in the time direction.¹⁻⁴ These enlarged lattices are then used to calculate hadronic correlation functions. The obvious gain of this trick is a possibility of a wider separation between a source and a sink corresponding to matter fields. It is, however, not clear whether this procedure is free of side effects distorting the particle spectrum. This important question has not received much attention so far. As a step towards clarifying the situation we consider in this Rapid Communication a quantum-mechanical example simple enough to be solved exactly or numerically with any desired precision.

Namely, let the problem be described by the Hamiltonian

$$H = \omega a^\dagger a - \lambda(a + a^\dagger)c^\dagger c, \tag{1}$$

where a and c correspond to boson and fermion degrees of freedom, respectively: $[a, a^\dagger] = \{c, c^\dagger\} = 1$, and ω is assumed to be positive. This is in fact a problem of a particle moving in a harmonic-oscillator potential with its spin $\frac{1}{2}$ coupled to a magnetic field. The latter is a linear function of the oscillator coordinate. One can easily verify the following expressions for the partition function

$$Z \equiv \text{Tr} e^{-\beta H} = \frac{1 + e^{\beta \frac{\lambda^2}{\omega}}}{1 - e^{-\beta \omega}} \tag{2}$$

and, for the fermion correlation function,

$$C(t) = \text{Tr}(c e^{-tH} c^\dagger e^{-(\beta-t)H}) = \exp \left[\frac{\lambda^2}{\omega^2} \left(\omega t + e^{-\omega t} - 1 + \frac{(1 - e^{-\omega t})^2}{1 - e^{-\omega \beta}} e^{-\omega(\beta-t)} \right) \right]. \tag{3}$$

The fermion effective mass is customarily defined as the logarithmic derivative of $C(t)$:

$$m_{\text{eff}} \equiv \frac{d}{dt} \ln C(t) = M \left(1 - \frac{\sinh \left[\omega \left(\frac{\beta}{2} - t \right) \right]}{\sinh \left(\frac{\omega \beta}{2} \right)} \right), \tag{4}$$

where

$$M \equiv \frac{\lambda^2}{\omega}. \tag{5}$$

The first term of Eq. (4) gives an energy gap M associated with the fermion. This quantity clearly represents the energy penalty for the spin pointing against the field direction. The second term is a finite-temperature correction apparently coming from the excited states of both the oscillator and the spin. In the low-temperature regime ($\beta\omega \gg 1$) this contribution is negligible if both $\beta - t$ and t are large compared to ω^{-1} , i.e., everywhere in the interval $0 \leq t \leq \beta$ except close vicinities of its edges.

With this simple physical picture in mind, we now

reformulate the problem in the path-integral language. This is most easily done using the holomorphic path-integral representation,^{5,6} giving for the partition function

$$Z = \left(\frac{1}{2\pi} \right)^n \int \prod_{m=0}^{n-1} dz_m d\bar{z}_m d\psi_m d\bar{\psi}_m e^S, \tag{6}$$

where the imaginary time interval β is split into n subintervals with pairs of c -number z, \bar{z} and anticommuting $\psi, \bar{\psi}$ variables corresponding to the intermediate points. In order for Eq. (6) to reproduce Eq. (2) periodic boundary conditions in time are to be assumed for z, \bar{z} and antiperiodic ones for $\psi, \bar{\psi}$. The action is

$$\begin{aligned} S &= S_F + S_B \\ &= \sum_{m=0}^{n-1} (e^g e^{f(\bar{z}_{m+1} + z_m)} \bar{\psi}_{m+1} \psi_m - \bar{\psi}_m \psi_m) \\ &\quad + \sum_{m=0}^{n-1} (e^{-\epsilon\omega} \bar{z}_{m+1} z_m - \bar{z}_m z_m), \end{aligned} \tag{7}$$

with the definitions $g \equiv (\frac{\lambda}{\omega})^2 (\epsilon\omega + e^{-\epsilon\omega} - 1)$, $f \equiv \frac{\lambda}{\omega} (1 - e^{-\epsilon\omega})$, and $\epsilon \equiv \frac{\beta}{n}$. Note that ϵ is not assumed to be

small, i.e., Z as given by Eq. (6) is independent of n and coincides with Eq. (2). The same should be true for the fermion correlation function, but, as will be shown in the following, using repeated field configurations leads to deviations persisting in both the continuum ($\epsilon \rightarrow 0$) and the zero-temperature ($\beta \rightarrow \infty$) limits.

Following the usual strategy we diagonalize the fermion matrix

$$\Lambda_1(l, m) \equiv e^g e^{f(\bar{z}_{m+1} + z_m)} \delta_{l, m+1} - \delta_{lm} \quad (8)$$

with the antiperiodicity condition imposed on the eigenvectors (the meaning of the subscript 1 will be clarified in the following). Being non-Hermitian, Λ_1 has different right and left eigenvectors. Namely, corresponding to every complex eigenvalue

$$\lambda_1^k = e^g \exp \left(\frac{f}{n} \sum_{j=0}^{n-1} (\bar{z}_j + z_j) - \frac{i\pi}{n} (2k+1) \right) - 1 \quad (k = 0, 1, \dots, n-1) \quad (9)$$

there are one right and one left eigenvectors with components

$$R_1^k(m) = \frac{1}{\sqrt{n}} \left(\frac{e^g}{1 + \lambda_1^k} \right)^m \exp \left(f \sum_{j=1}^m (\bar{z}_j + z_{j-1}) \right) \quad (10)$$

and $L_1^k(m) = [nR_1^k(m)]^{-1}$, accordingly. The fermions can now be integrated out and e^{S_F} in Eq. (6) replaced by

$$\det \Lambda_1 = \prod_{k=0}^{n-1} \lambda_1^k = 1 + e^{ng} \exp \left(f \sum_{j=0}^{n-1} (\bar{z}_j + z_j) \right). \quad (11)$$

Note that this substitution and integration over z, \bar{z} indeed recovers Eq. (2).

To study the effect of the repeated N times z field configuration one must replace the $n \times n$ matrix Λ_1 by the $nN \times nN$ matrix Λ_N whose definition is identical to Eq. (8) but it is understood that l, m now run from 0 to $nN - 1$, while the z field is still periodic with period n . The eigenvalues of this new matrix are

$$\lambda_N^k = e^g \exp \left(\frac{f}{n} \sum_{j=0}^{n-1} (\bar{z}_j + z_j) - \frac{i\pi}{nN} (2k+1) \right) - 1 \quad (k = 0, 1, \dots, nN-1), \quad (12)$$

and the eigenvectors are given by Eq. (10) with λ_1 replaced by λ_N . It is now straightforward to derive the fermion correlation function. The first step is inversion of Λ_N :

$$\Lambda_N^{-1}(l, m) = \sum_{k=0}^{nN-1} \frac{1}{\lambda_N^k} R_N^k(m) L_N^k(l) = \sum_{k=0}^{nN-1} (1 + \lambda_N^k)^{l-m} e^{(m-l)g} \frac{1}{\lambda_N^k} \exp \left(f \sum_{l+1}^m (\bar{z}_j + z_{j-1}) \right) \quad (13)$$

(it is assumed for the definiteness that $0 < l < m < n$). The summation over k involves some simple algebra leading to

$$\Lambda_N^{-1}(l, m) = \frac{e^{g(m-l)} \exp \left(f \sum_{j=l+1}^m (\bar{z}_j + z_{j-1}) \right)}{1 + \exp \left(N f \sum_{j=0}^{n-1} (\bar{z}_j + z_j) \right)}. \quad (14)$$

The denominator of the last expression is just $\det \Lambda_N$, as expected. Thus if the repeated z field configuration is used the fermion correlation function is

$$C_N(l, m) = \int \prod_{i=0}^{n-1} dz_i d\bar{z}_i e^{g(m-l)} \exp \left(f \sum_{j=l+1}^m (\bar{z}_j + z_{j-1}) \right) \frac{\det \Lambda_1}{\det \Lambda_N} e^{S_B}. \quad (15)$$

Obviously, $C_N(l, m)$ considerably simplifies for $N = 1$. In the latter case, the result Eq. (3) is recovered upon the integration over \bar{z}, z , and the dependence on the lattice spacing ϵ disappears. This is no longer the case for the arbitrary N , as can be shown in the following simple way. Among all the Fourier components of the z field the N dependence of Eq. (15) comes only from the integration over the zero-frequency component appearing in $\det \Lambda_N$. Thus C_N/C_1 is just the ratio of one-dimensional integrals:

$$\frac{C_N(l, m)}{C_1(l, m)} = \frac{F_N(l, m)}{F_1(l, m)}, \quad (16)$$

where

$$F_N(l, m) \equiv \int dx \frac{1 + e^{ng} e^{2f\sqrt{nx}}}{1 + e^{nNg} e^{2Nf\sqrt{nx}}} e^{(m-l)g} \exp \left(-\frac{\omega f}{\lambda x^2} + \frac{2}{\sqrt{n}} (m-l)x \right) \quad (17)$$

and

$$x \equiv \frac{1}{2\sqrt{n}} \sum_{j=0}^{n-1} (\bar{z}_j + z_j). \quad (18)$$

The ratio Eq. (16) is most easily analyzed if the copying process is pushed to its extreme: $N \rightarrow \infty$. In this case the denominator of Eq. (17) is replaced by the step function of $ng + 2f\sqrt{n}x$. Integrating Eq. (17) gives, for the ratio Eq. (16),

$$\frac{C_\infty(l, m)}{C_1(l, m)} = e^{-P_0^2} \sum_{q=0}^1 e^{P_q^2} \text{erfc}(P_q), \quad (19)$$

where

$$P_q \equiv \sqrt{\frac{\lambda f n}{\omega}} \left(\frac{\omega g}{2f\lambda} + \tau + q \right) \quad (20)$$

with $\tau \equiv \frac{m-l}{n} = \frac{t}{\beta}$, and erfc denotes the complementary error function. Evidently, the ratio Eq. (19) is n (or ϵ) dependent. Moreover, $C_\infty(l, m)$ does not in general approach $C_1(l, m)$ in the continuum limit $\epsilon \rightarrow 0$. In the latter case g must be replaced by 0 and f by $\epsilon\lambda$, and therefore

$$P_q \rightarrow b(\tau + q) \quad (21)$$

with the notation $b \equiv \lambda\sqrt{\frac{\beta}{\omega}}$. Substituting Eq. (21) into Eq. (19) and taking the logarithmic derivative gives the continuum-limit correction to the effective mass [cf. Eq. (5)]:

$$\Delta m_{\text{eff}} = \frac{2M}{b} \left(\frac{be^{b^2(\tau+1)^2} \text{erfc}[b(\tau+1)] - 1}{e^{b^2\tau^2} \text{erfc}(b\tau) + e^{b^2(\tau+1)^2} \text{erfc}[b(\tau+1)]} \right). \quad (22)$$

This correction has the following properties.

(i) In the high-temperature regime ($b \ll 1$) Δm_{eff} can be expanded in powers of b leading to

$$\Delta m_{\text{eff}} = -\frac{2M}{b} \left(1 - b + \frac{2b}{\sqrt{\pi}} (2\tau + 1) \right). \quad (23)$$

This is a very large negative correction slowly varying with τ . It is therefore impossible to deduce the value of M from m_{eff} measured in the high-temperature regime: the physics of the model is completely obscured by the finite-size effect due to the copying.

(ii) In the low-temperature regime⁷ ($b \gg 1$) there are two possibilities depending on the value of τ . For $b\tau \gg 1$ the error functions can be replaced by their asymptotic expressions giving

$$\Delta m_{\text{eff}} = -2M\sqrt{\pi} \frac{\tau \left(\tau + 1 + \frac{1}{\sqrt{\pi}} \right)}{2\tau + 1}. \quad (24)$$

This correction is several times larger than M itself, and again m_{eff} measured in this region yields little use-

ful information. The situation is considerably better for $b\tau \gg 1$. Expanding $\text{erfc}(b\tau)$ in powers of $b\tau$ and taking the asymptotic expression for $\text{erfc}[b(\tau+1)]$ one obtains

$$\Delta m_{\text{eff}} = -\frac{2M}{b} \left(1 + \frac{1}{\sqrt{\pi}} \right) \left(1 + \frac{2b\tau}{\sqrt{\pi}} \right). \quad (25)$$

Obviously, this time Δm_{eff} is well under control, making $b \gg 1$, $b\tau \gg 1$ the only useful region for measuring M .

The case of finite N is technically more difficult to analyze, but the results are qualitatively similar to those for $N = \infty$. Expanding the denominator of the integrand in Eq. (17) in powers of $e^{nNg} e^{2Nf\sqrt{n}x}$ and integrating over x one finds

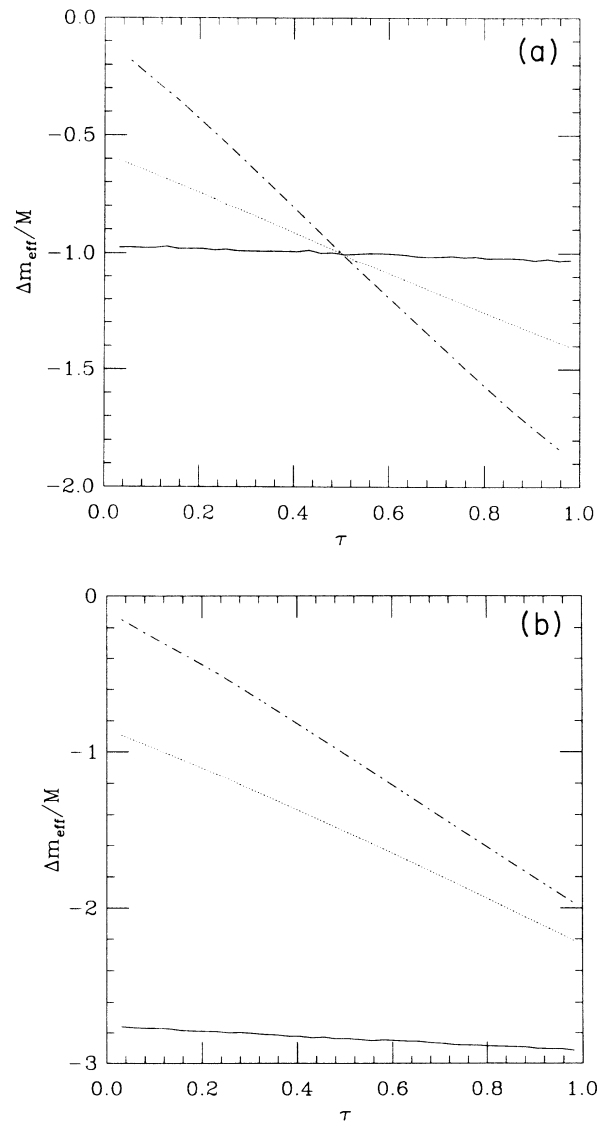


FIG. 1. (a) Imaginary-time dependence of the relative effective-mass correction $\Delta m_{\text{eff}}/M$ due to doubling ($N = 2$) for $b = 0.1$ (solid line), 1 (dotted line), and 10 (dashed-dotted line). (b) Corresponding dependence due to quadrupling ($N = 4$).

$$\frac{C_N(l, m)}{C_1(l, m)} = e^{-P_0^+(0)^2} \sum_{k=0}^{\infty} \sum_{q=0}^1 (-1)^k \{ e^{P_q^+(k)^2} \operatorname{erfc}[P_q^+(k)] + e^{P_q^-(k+1)^2} \operatorname{erfc}[P_q^-(k+1)] \}, \quad (26)$$

where, similarly to Eq. (20),

$$P_q^{\pm}(k) \equiv \sqrt{\frac{\lambda f n}{\omega}} \left[kN \pm \left(\frac{\omega g}{2f\lambda} + \tau + q \right) \right]. \quad (27)$$

Again the n dependence of $C_N(l, m)$ clearly shows up in Eqs. (26) and (27). In the continuum limit,

$$P_q^{\pm}(k) \rightarrow b[kN \pm (\tau + q)]. \quad (28)$$

These continuum-limit expressions for $P_q^{\pm}(k)$ are assumed in the following.

There is no obvious way of summing the series Eq. (26) analytically. Numerically the series is found to be slowly convergent. The convergence is much improved using Cesaro's summation by arithmetic means. With the eighth term included, the truncation error in Δm_{eff} is within $0.03M$ in a wide range of all the involved parameters for $N = 1$ (where the exact value of Δm_{eff} is 0), 2, or 4. Such an accuracy is good enough for understanding the effect of the multiple z field configurations on the fermion correlation function. As shown in Fig. 1, the behavior of Δm_{eff} for finite N follows the pattern found for $N = \infty$, restricting the region for the M measurement to the narrow window $b \gg 1$, $b\tau \ll 1$. The latter point is further stressed in Fig. 2 where $\Delta m_{\text{eff}}/M$ is plotted against b^{-1} for $b\tau = 0.1$. These curves are in good qualitative agreement with Eq. (25): Δm_{eff} approaches 0 with b ; the curves would not change considerably if a different small value of $b\tau$ were chosen.

Two features of the correlation function Eq. (15) are

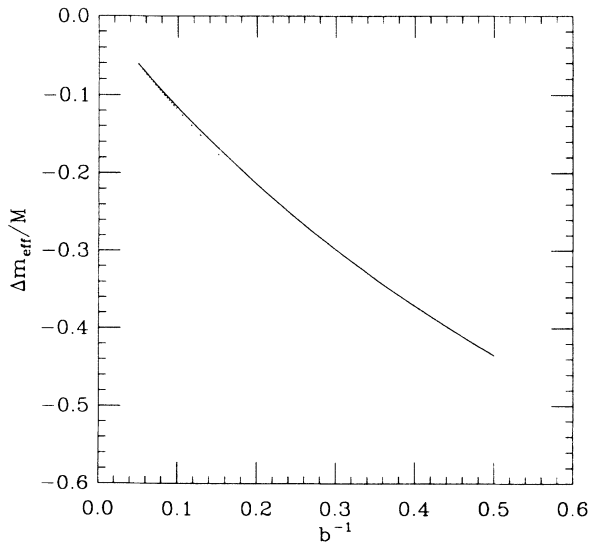


FIG. 2. Relative effective-mass correction $\Delta m_{\text{eff}}/M$ plotted against b^{-1} for $b\tau = 0.1$. The N values are 2 (solid line) and 4 (dotted line).

essential to yield the behavior we found for Δm_{eff} . First of all, $\det\Lambda_N$ in the denominator suppresses the ground-state configurations of the z field. For $N > 1$ this suppression cannot be completely compensated by $\det\Lambda_1$ in the numerator. As a result, the ground-state energy is effectively increased, and the correction to the fermion energy gap should therefore be negative. The nearly linear variation of Δm_{eff} can be traced back to the fact that only the zero-frequency component of the z field is important for the fermion dynamics. It then follows from Eqs. (16) and (17) that the multiplicative correction to the correlation function is approximately Gaussian. Both these features might be found in more realistic models.

Finally, we consider the interplay between the finite-temperature effect of Eq. (4) on one hand, and the configuration copying, on the other. In a certain range of parameters b and ω (there is no restriction on b if $\beta\omega \rightarrow \infty$) the behavior of m_{eff} (including the Δm_{eff} correction) exhibits a wiggle as shown in Fig. 3. This shape of the effective mass curve is very similar to those found for mesons on doubled and quadrupled lattices in a recent QCD calculation.⁴ It seems plausible that in either case the peculiarities of the m_{eff} curve have a common origin.⁸ As far as the M measurement is concerned, the overlap of the two corrections is unfortunate: while Δm_{eff} may become small only in the vicinity of $\tau = 0$, this is exactly where the correction of Eq. (4) is of order M .

The lessons learned from this simple example can be summarized as follows. Copying field configurations results in a time-dependent (roughly linear) correction to

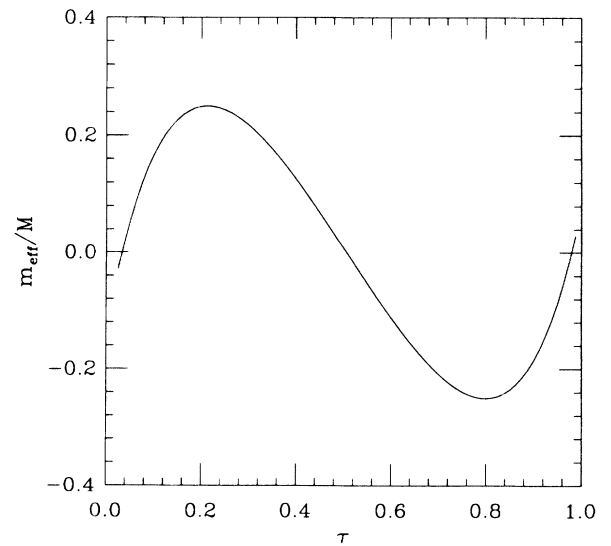


FIG. 3. Imaginary-time dependence of m_{eff}/M for $b = 10$ and $\beta\omega = 5.5$ (doubled configuration).

the fermion effective mass. At low temperatures this correction is large compared to the exact mass value except for the times much shorter than the inverse temperature. Thus the configuration copying may miss its original goal: longer time separation in the correlation function. The correction arising from the copying may lead to an oscillatory behavior of the effective mass, similar to the one observed in QCD on doubled lattices. This might indicate that the described mechanism is indeed not strongly

model dependent. If so, the virtue of the configuration copying is far from obvious, and this technique should be applied with caution.

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⁷Note that the finite-temperature effect due to copying has M^{-1} as its typical time scale. This is different from ω^{-1} , the typical finite-temperature time scale of Eq. (4).

⁸A different explanation of this phenomenon in QCD has been proposed by D.K. Sinclair (private communication): the oscillatory behavior of the meson propagator is attributed to the interference of the quark correlation functions with different boundary conditions. That model differs from the current work in two aspects: it assumes periodic boundary conditions for the fermions on an enlarged lattice and disregards excited states.