Application of the semiquantum approximation to lattice field theories

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We show that the semiquantum approximation to energy levels of simple lattice field theories using site variables gives results in agreement with those obtained with collective modes.

In recent papers a semiquantum method to evaluate energy levels[1] has been applied to lattice field theories.[2] This method consists of replacing the kinetic part of the Hamiltonian with a function of the coordinate which contains some parameters. The energy eigenvalue is obtained by minimizing with respect to the coordinate and maximizing with respect to the parameters. It has been shown in Ref. 2 that a satisfactory approximation to the energy eigenvalues of field theories is obtained by using the collective variables which diagonalize the intersite interactions.

The purpose of this note is to point out that reasonable results may also be reached with site variables, provided a suitable parametrization is given for the kinetic terms.

Let us begin with the free-scalar-field case. The essential aspect of the problem may be seen by considering just the two-site Hamiltonian

$$H=\sum_{i=1}^{2}\left(\frac{p_i^2}{2}+\frac{M^2}{2}\phi_i^2\right)+\tfrac{1}{2}(\phi_2-\phi_1)^2\,, \tag{1}$$

where p_i are the momenta conjugate to the fields ϕ_i at sites i, and the gradient term is approximated by the difference of field values. It is obvious that by introducing collective variables

$$\xi_1=\frac{1}{\sqrt{2}}(\phi_1+\phi_2),\quad \xi_2=\frac{1}{\sqrt{2}}(\phi_1-\phi_2) \tag{2}$$

the Hamiltonian in Eq. (1) is diagonalized giving

$$H=\sum_{n=1}^{2}\left(\frac{\pi_n^2}{2}+\frac{(M^2+k_n^2)}{2}\xi_n^2\right), \tag{3}$$

where $k_1=0$ and $k_2=\sqrt{2}$.

The semiquantum (SQ) approximation consists in general of replacing the kinetic term by

$$\pi^2=\frac{1}{4}\left(\frac{g'(\xi)}{g(\xi)}\right)^2. \tag{4}$$

If the wave function $\Psi(\xi)$ were known, the energy eigenvalue would be given by the choice $g=\Psi'/\Psi$ and a minimization with respect to ξ. It is therefore convenient to represent g by

$$g(\xi)=\frac{\prod_m(\xi-\xi_m)}{\prod_z(\xi-\xi_z)}\,, \tag{5}$$

where ξ_m and ξ_z are the wave-function maxima and zeros, respectively. Guessing the number of maxima and zeros for a particular level, the approximate energy is obtained by varying the parameters ξ_m and ξ_z until the highest value of the minimum of the Hamiltonian as a function of the coordinate is reached.

Applying the SQ method to Eq. (3), it is clear that by having the ground-state wave function with one maximum at the origin of the collective variable ξ_n and no zeros, the SQ approximation is

$$\pi_n^2=\frac{1}{4\xi_n^2}\,. \tag{6}$$

Minimizing Eq. (3) with respect to ξ_n, one obtains in this case the exact result $E=\sum_n\frac{1}{2}(M^2+k_n^2)^{1/2}$.

Returning to the Hamiltonian Eq. (1), if we use the SQ method for site variables

$$p_i^2=\frac{1}{4\phi_i^2}\,, \tag{7}$$

the minimization with respect to ϕ_i corresponds to $\phi_1=\phi_2$ and $E=\sum_{i=1}^{2}\frac{1}{2}M$, a result which, as noted in Ref. 2, is due to the fact that only the mode with wave vector $k_1=0$ survives.

We wish to remark that approximation Eq. (7) comes from the assumption that the wave function for each site is centered around $\phi_i=0$. It is, however, sensible to think that both wave functions must be shifted because of the mutual interaction giving the approximation

$$H_{SQ}=\sum_{i=1}^{2}\left(\frac{1}{8(\phi_i-A_i)^2}+\frac{M^2+1}{2}\phi_i^2\right)-\phi_1\phi_2\,. \tag{8}$$

In Fig. 1 we represent each single-site part of H_{SQ} for $A_1=-A_2$, i.e., without the term $-\phi_1\phi_2$. It is clear that for a particular value of the parameter three minimal configurations can be made equal, (a_1a_2), (b_1b_2), and (a_1b_2) corresponding to

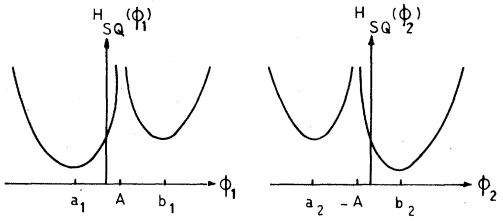

FIG. 1. Free field. $H_{SQ}(\phi_i)$ represent the single-site parts of Eq. (8).

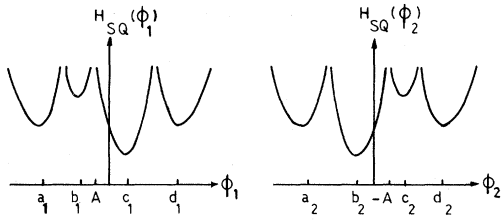

FIG. 2. Quartic self-interaction. $H_{SQ}(\phi_i)$ represent the single-site parts of Eq. (10).

having both coordinates in the left well, both in the right, and the first in the left and the second in the right. In fact, the larger single-site energy of the first two configurations is compensated by their negative intersite interaction. The presence of configurations with nonequal ϕ_1 and ϕ_2 gives rise to contributions of both normal modes. The equal energy of these configurations maximizes the minima of H_{SQ} attainable with this parametrization. The numerical calculation indicates that for a weak coupling ($M=3$) the exact result $E=3.158$ is well approximated by the SQ method applied to site variables which gives $E=3.111$ for $A=0.038$, whereas with Eq. (7) the low value $E=3.0$ is obtained. For strong intersite coupling ($M=0.5$) the SQ approximation is not so good since it gives $E=0.629$ for $A=0.48$ compared to the exact value $E=1.0$ and the one coming from Eq. (7) which is $E=0.5$. This occurs because the wave function for each site is not suitably represented by a simple shifted distribution with only a maximum when the value of A turns out to be large.

Looking now at a case where neither the site variables nor the collective ones diagonalize the Hamiltonian, the outcome is that the SQ method applied to both sets gives similar results. To show this, we analyze a scalar field with a two-minima potential, again restricting to the two-site system

$$H=\sum_{i=1}^{2}\left[\frac{p_i^2}{2}+\lambda(\phi_i^2-f^2)^2\right]+\tfrac{1}{2}(\phi_2-\phi_1)^2. \tag{9}$$

We may replace the kinetic terms by the functions of the fields corresponding, for each site, to a wave function with maxima around the minima of the potential and a zero near the maximum of the barrier. Therefore for $\lambda=1$ and $f^2=1.5$ we take the parametrization for the ground state

$$H_{SQ}=\sum_{i=1}^{2}\left[\frac{1}{8(\phi_i-A_i)^2}\left(\frac{\phi_i^2+B_i}{\phi_i^2-B_i}\right)^2+(\phi_i^2-1.5)^2\right]$$
$$+\tfrac{1}{2}(\phi_2-\phi_1)^2. \tag{10}$$

Now each single-site part of Eq. (10) has four minima, as shown in Fig. 2 where for reasons of symmetry the zeros of the wave functions have been chosen $A_1=-A_2$ and the maxima $B_1=B_2$. Maximizing with respect to these two free parameters, it is possible to make equal the minimal energy configurations (a_1a_2), (a_1b_2) and their symmetric counterparts (d_1d_2), (c_1d_2). The energy turns out to be $E=3.90$ for $B=1.56$ and $A=0.07$, quite close to the result $E=3.83$ for $A=0.07$ obtained when B is kept fixed to the value 1.54 which corresponds to the minimum of energy of a single-site Hamiltonian, showing that A is the most relevant parameter.

Introducing the collective variables Eq. (2) which diagonalize the intersite term, the Hamiltonian Eq. (9) may be written as

$$H=\tfrac{1}{2}\pi_1^2+\tfrac{1}{2}\pi_2^2+\xi_2^2+\lambda(\phi_1^2-f^2)^2+\lambda(\phi_2^2-f^2)^2. \tag{11}$$

Its classical solution is $\phi_1=\phi_2=\pm f$, i.e., $\xi_1=\sqrt{2}f$, $\xi_2=0$, and the conjugate momenta $\pi_1=\pi_2=0$, which corresponds to zero energy. If we apply the SQ method in the simplest way to avoid this classical configuration

$$\pi_1^2=\frac{1}{4(\xi_1-\sqrt{2}f)^2},\quad \pi_2^2=\frac{1}{4\xi_2^2}, \tag{12}$$

the resulting energy turns out to be $E=1.84$ which is clearly too low. The reason is that prescription Eq. (12) corresponds to a wave function in ξ_n with only one maximum, whereas rewriting the quartic potential of Eq. (11) in terms of ξ_n a quartic potential appears again. Since this potential has two minima as in the site case, one must choose a prescription for the kinetic terms which corresponds to a ground-state wave function with two maxima and one zero, i.e.,

$$H_{SQ}=\sum_{n=1}^{2}\left[\frac{1}{8(\xi_n-A_n)^2}\left(\frac{\xi_n^2+B_n}{\xi_n^2-B_n}\right)^2\right]+\tfrac{1}{2}\xi_1^4-3\xi_1^2$$
$$+\tfrac{1}{2}\xi_2^4-2\xi_2^2+3\xi_1^2\xi_2^2+4.5. \tag{13}$$

Taking $A_1=A_2=0$ since the intersite term does not break the symmetry $\xi_n\to-\xi_n$, the optimum value is $E=3.80$ for $B_1=2.56$ and $B_2=1.56$, which is quite close to the one calculated with the sites in Eq. (10). We note that because of the numerical

value of B_1 the configuration corresponding to the classical solution of Eq. (11) is avoided in this case, too. The conclusion is that a simple way to apply the SQ method is to write the Hamiltonian in terms of site or collective variables and replace the kinetic terms by functions suggested by the eigenfunction of the single-site (-mode) Hamiltonian allowing small shifts in the parameters to be used to maximize the minimal energy configurations. With both choices the number of free parameters is equivalent.

Having shown that the calculations with site or collective variables give similar results, for larger number of sites the site prescription is more convenient because of its greater simplicity. This is because it is not necessary to diagonalize the intersite terms and all the site potentials are equal. To limit the number of parameters necessary to evaluate the ground-state energy, one may keep the maxima of the wave function B_i fixed to the one-site value and vary the position of zeros A_i. It turns out that the optimum values for a free end-point chain correspond to smooth changes of A_i from A_1 to $A_N = -A_1$. For $N = 3$, e.g., this means $A_1 = -A_3$ and $A_2 = 0$.

Similar calculations with the site variables may be performed for a closed ring with periodic $\phi_{N+1} = \phi_1$ or antiperiodic $\phi_{N+1} = -\phi_1$ conditions, the former corresponding to the vacuum and the latter to a kink solution. It turns out that this site procedure gives values quite close to the ones obtained in Ref. 2 where the displacement with respect to the classical solutions had been used as variables for the SQ method. E.g., already for $N = 3$, and $\lambda = 1$, $f^2 = 1.5$, our site prescription gives an energy per site of 2 for the vacuum and 2.3 for the kink configuration, whereas in Ref. 2 the calculation for $N = 8$ gave 2.3 and 2.4, respectively.

We have shown that the SQ method with site variables represents a quick procedure to compute approximate energy levels of simple lattice field theory. This is the only version which can be practically used in cases where the diagonalization of the intersite terms is quite complicated as in the Reggeon field theory.[3]

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