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Semiclassical Fluctuations in the Quantum Phase Model

Mahn-Soo CHOI*, T. I. UM and M. Y. CHOI

Department of Physics and Center for Theoretical Physics, Seoul National University, Seoul 151-742

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We consider the one-dimensional quantum phase model coupled to a thermal bath at finite temperatures and investigate the competition of quantum and thermal fluctuations. By means of a variational method, we obtain the effective classical Hamiltonian, which manifests a crossover from quantum to classical behaviors of the fluctuations. It is also shown that the peculiar nature of the quantum-phase model restricts the applicability of the otherwise well-working variational method to a certain range of quantum fluctuations.

I. INTRODUCTION

In a recent breakthrough in our understanding of ultra-small tunnel junctions and arrays, as well as granular superconductors, the quantum-phase model (QPM) has served as a fundamental model, incorporating both the charging energy and the Josephson-coupling energy which compete with each other and which bringing about strong quantum fluctuations at low temperatures [1]. Because of the quantum fluctuations, the QPM is now well known to exhibit quantum phase transitions at zero temperature, such as the superconductor-insulator transitions in Josephson-junction arrays (JJAs) [2–4]. Although, in its precise meaning, the quantum phase transition, occurs only at zero temperature, quantum fluctuations often survive and play significant roles even at finite (albeit sufficiently low) temperatures, and the interplay of the quantum and the thermal fluctuations have already been the source of a number of experimental and theoretical works [5]. Amongst them is a semiclassical approach to the QPM based on the Giachetti-Tognetti-Feynman-Kleinert (GTFK) variational method [6], addressing the issue of reentrance behavior in two-dimensional (2D) JJAs at very low temperatures [7]. Unlike previous works, which are essentially mean-field in nature, this approach has attracted considerable attention, partly because of the great success of the underlying GTFK method applied to various potentials and partly due to the lack of an adequate method to account for *both* the quantum and the thermal fluctuations satisfactorily. Indeed, this approach applied to 2D arrays has predicted transitions of the Berezinskii-Kosterlitz-Thouless type for weak quantum fluctuations, which may not be obtained via the mean-field approach, and has produced results at low temperatures consistent with the known zero-temperature results [7].

The purpose of this paper is two fold: On the one hand, we formulate the GTFK variational method applied to the QPM more thoroughly than in Ref. [7] (to be referred to as KKC in the following) and examine the validity of the method in this particular model, which was not properly considered in KKC. The motivation is that the QPM provides an example of a potential that puts a rather strong restiction on the applicability of the GTFK method. On the other hand, we investigate the competition between the quantum and the thermal fluctuations in the one-dimensional (1D) QPM, having in mind 1D arrays of ultra-small Josephson junctions at finite temperature, within the restricted, but still interesting, region of the parameter space where the GTFK method is valid. Notwithstanding its importance in view of experiments, there have been few studies of the finite-temperature effects in the 1D QPM, which contrasts with the numerous works performed in two dimensions.

To consider the GTFK method from a more fundamental point of view, we begin in Sec. with a single phase variable describing, *e.g.*, a single Josephson junction. This reveals that the peculiar nature of the QPM restricts the applicability of the otherwise well-working variational method to a certain limited range of quantum fluctuations. Section investigates the finite-temperature effects in the 1D QPM. It is found that quantum fluctuations survive at sufficiently low, but finite, temperatures and play significant roles, renormalizing the potential strength substantially. Finally, Sec. concludes the paper and gives a brief discussion of the experimental situation as well.

II. SINGLE PHASE VARIABLE

*Present address: Korea Institute for Advanced Study, Cheonryangri-dong 207-43, Seoul 130-012

In this section, we introduce the QPM with a single phase variable and apply the GTFK variation method, which leads to the effective classical potential for the system. Since the detailed procedure is already well established in the literature [8], we here sketch briefly the procedure, albeit making clear the nature of the approach and pointing out the peculiarity of the QPM.

In the imaginary-time path-integral formalism, the QPM with the single phase variable φ is described by the Euclidean action:

$$S_0/\hbar \equiv \beta J \int_0^{\hbar\beta} \frac{d\tau}{\beta\hbar} \left[\frac{1}{2\omega_p^2}\dot{\varphi}(\tau)^2 - \cos\varphi(\tau)\right], \qquad (1)$$

where J is the height of the periodic potential and ω_p is the characteristic frequency of the dynamics of the phase variable. For convenience, we also define $\alpha \equiv \hbar\omega_p/J$, the ratio of the energy of the quantum zero-point motion to the potential energy, which measures the strength of the quantum fluctuations. In the case of a Josephson junction, for instance, J is the Josephson-coupling energy, $\omega_p \equiv \sqrt{8E_C J}/\hbar$, with E_C being the charging energy, is the Josephson-plasma frequency of the junction, and α is given by the ratio of the charging energy to the Josephson energy: $\alpha = \sqrt{8E_C/J}$.

When the phase variable is coupled to a thermal bath at temperature $1/\beta$, on the other hand, there appears an additional effective dissipative action. In the Caldeira-Leggett (CL) model [9], the dissipative action reads

$$S_D/\hbar \equiv \beta J \sum_{n=1}^{\infty} \left(\gamma\omega_n/\omega_p^2\right) |\varphi_n|^2, \qquad (2)$$

where γ is the damping coefficient and φ_n ($n = 0, 1, 2, \cdots$) is the Fourier component

$$\varphi(\tau) \equiv \varphi_0 + \sum_{n=1}^{\infty} \left[\varphi_n e^{-i\omega_n\tau} + \text{c.c.}\right] \qquad (3)$$

corresponding to the thermal frequency $\omega_n \equiv 2\pi n/\beta\hbar$. In general, the physical origin of the dissipation, which is inevitable at finite temperatures, varies with the details of the system described by the QPM and with the actual coupling of the phase variable to the thermal bath. For example, in Josephson-junction systems, the major source of dissipation is quasiparticle tunneling whereas the shunt resistance plays a dominant role in superconducting point contacts or constrictions. Such details are, however, not essential in the following formulation (see Ref. [10]), and we here adopt for simplicity the CL model given by Eq. (2), which is widely believed to describe well Ohmic dissipation. It should also be pointed out that without such a dissipation, the contributions from the paths with non-zero winding numbers, $\varphi(\beta\hbar) = \varphi(0) + 2\pi\ell$ for $\ell = 0, 1, 2, \cdots$, are crucial [11]. Since the winding number contribution is beyond the scope of this work, we henceforth put $\ell = 0$ and further focus on the case of weak dissipation: $\gamma \ll \omega_0$.

In terms of the Fourier decomposition in Eq. (3) and the integration measure for the non-zero frequency components [8]

$$\int d\{\varphi_n\varphi_n^*\} \equiv \int_{-\infty}^{\infty} \prod_{n=1}^{\infty} \left[\int \frac{d\varphi_n d\varphi_n^*}{2\pi i\omega_p^2/\beta J\omega_n^2}\right],$$

the partition function for the QPM in Eqs. (1) and (2) takes the form

$$Z = \int \frac{d\varphi_0}{\sqrt{2\pi\beta\hbar^2\omega_p^2/J}} \exp[-\beta H_{cl}(\varphi_0)], \qquad (4)$$

where the effective classical Hamiltonian has been defined according to

$$\exp[-\beta H_{cl}(\varphi_0)] \equiv \int d\{\varphi_n\varphi_n^*\} \exp\left\{-\frac{1}{\hbar}S[\varphi(\tau)]\right\} \qquad (5)$$

with the total action $S \equiv S_0 + S_D$. Since it is not possible to compute exactly the effective classical Hamiltonian, we employ the GTFK approach and choose a trial action of the form

$$\frac{S_1}{\hbar} = \frac{\beta J}{2\omega_p^2} \sum_{n=1}^{\infty} \left[\omega_n^2 + \gamma\omega_n + \Omega^2(\varphi_0)\right] |\varphi_n|^2, \qquad (6)$$

which corresponds to the replacement of the cosine potential in Eq. (1) with the harmonic potential

$$-\cos[\varphi(\tau)] \approx \left[\frac{\Omega^2(\varphi_0)}{2\omega_p^2}\right] [\varphi(\tau) - \varphi_0]^2.$$

The φ_0-dependent frequency $\Omega(\varphi_0)$ is to be determined in a variational manner as follows: The convexity of the exponential function leads to the Jensen-Peierls inequality

$$\exp[-\beta H_{cl}(\varphi_0)] \geq \exp\left\{-\beta H_{cl}^1(\varphi_0) - \frac{1}{\hbar}\langle\, S - S_1 \,\rangle_{S_1,\varphi_0}\right\}, \qquad (7)$$

where $\exp[-\beta H_{cl}^1] \equiv \int d\{\varphi_n\varphi_n^*\} \exp[-S_1/\hbar]$ and the average with respect to the trial action for φ_0 is defined by

$$\langle \cdots \rangle_{S_1,\varphi_0} \equiv \frac{\int d\{\varphi_n\varphi_n^*\} e^{-S_1/\hbar}[\cdots]}{\int d\{\varphi_n\varphi_n^*\} e^{-S_1/\hbar}}.$$

In other words, we have the upper bound $H_{cl}^*(\varphi_0)$ for the *true* effective classical Hamiltonian $H_{cl}(\varphi_0)$:

$$H_{cl}(\varphi_0) \leq H_{cl}^*(\varphi_0) \equiv H_{cl}^1(\varphi_0) + \frac{1}{\hbar\beta}\langle\, S - S_1 \,\rangle_{S_1,\varphi_0}. \qquad (8)$$

As a result, we can determine $\Omega(\varphi_0)$ by minimizing $H_{cl}^*(\varphi_0)$ so that $H_{cl}^*(\varphi_0)$ becomes the optimal upper bound and thus provides a very good approximation to the true effective classical potential $H_{cl}(\varphi_0)$ over a wide range of temperatures. This yields the coupled equations for the variational parameter:

$$\Omega^2(\varphi_0) = \omega_p^2 \exp\left[-a^2(\varphi_0)/2\right] \cos\varphi_0 \qquad (9)$$

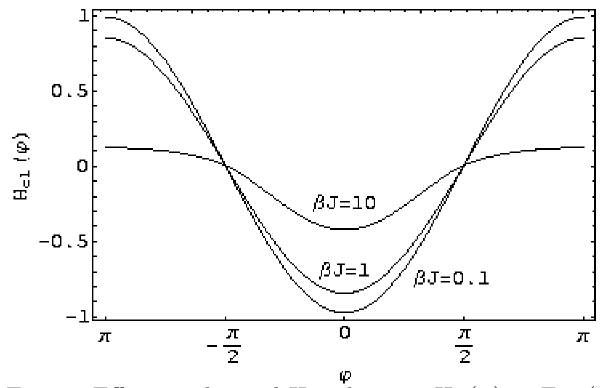

Fig. 1. Effective classical Hamiltonian $H_{cl}(\varphi)$ in Eq. (12) at three different temperatures, $\beta J = 10, 0$, and $1/10$, for $\alpha = 1$ and $\gamma = 0.05\omega_p$.

and

$$a^2(\varphi_0) \equiv \frac{2\omega_p^2}{\beta J}\sum_{n=1}^{\infty}\frac{1}{\omega_n^2+\gamma\omega_n+\Omega^2(\varphi_0)}, \tag{10}$$

which in turn leads to the optimal upper bound for the effective classical Hamiltonian

$$\begin{aligned} H_{cl}(\varphi) &= -Je^{-a^2(\varphi)/2}\left[1+a^2(\varphi)/2\right]\cos\varphi \\ &\quad -\frac{1}{\beta}\sum_{n=1}^{\infty}\ln\frac{\omega_n^2}{\omega_n^2+\gamma\omega_n+\Omega^2(\varphi)}. \end{aligned} \tag{11}$$

Here the asterisk in H^*_{cl}, as well as the subscript 0 in φ_0, has been omitted for simplicity. More explicitly, putting $\gamma = 0$ in the weak-dissipation limit (see below), one gets

$$\begin{aligned} H_{cl}(\varphi) &= -Je^{-a^2(\varphi)/2}\left[1+a^2(\varphi)/2\right]\cos\varphi \\ &\quad -\frac{1}{\beta}\ln\frac{\beta\hbar\Omega(\varphi)/2}{\sinh[\beta\hbar\Omega(\varphi)/2]}, \end{aligned} \tag{12}$$

together with

$$a^2(\varphi) = \frac{1}{4}\alpha^2\beta J F[\beta\hbar\Omega(\varphi)/2], \tag{13}$$

where $F(x) \equiv x^{-2}(x\coth x - 1)$. Figure 1 shows the general behavior of the effective classical Hamiltonian as a function of φ at three different temperatures. It can be observed that quantum fluctuation effects become significant as the temperature is lowered, yielding marked deviations from the cosine-type potential at low temperatures ($\alpha\beta J \gg 1$).

Apart from the additional φ-dependence of the front factor $Je^{-a^2(\varphi)/2}[1 + a^2(\varphi)/2]$, the effective classical Hamiltonian in Eq. (12) is reminiscent of the Hamiltonian for a macroscopic (classical) junction. Naturally, the extent of the φ-dependence here depends on the strength α of the quantum fluctuations. Indeed, in the high-temperature classical limit ($\alpha\beta J \to 0$), it is obvious that Eq. (12) reduces to

$$H_{cl}(\varphi) \simeq -J\cos\varphi.$$

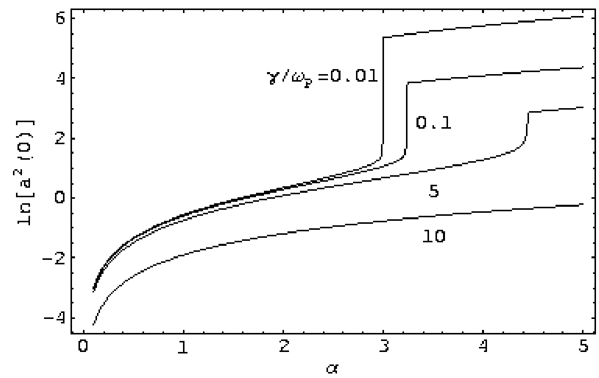

Fig. 2. Optimal values of the variational parameter $a^2(0)$ versus α for $\gamma/\omega_p = 0.01, 0.1, 5$, and 10 at (low) temperature $\beta J = 0.001$.

In the opposite low-temperature limit ($\alpha\beta J \to \infty$), on the other hand, the effective classical Hamiltonian in Eq. (12) is ill-behaving, as can be seen from the effective potential height

$$\begin{aligned} \Delta U_{cl} &\equiv H_{cl}(\pi) - H_{cl}(0) \\ &= \begin{cases} Je^{-a^2(0)/2}\left[1-\dfrac{2}{e}\dfrac{\alpha}{\alpha_c}\right], & \alpha < \alpha_c \\ Je^{-\alpha^2\beta J/24} \to 0, & \alpha > \alpha_c \end{cases} \end{aligned} \tag{14}$$

with

$$a^2(0) \approx \begin{cases} \dfrac{4}{e}\dfrac{\alpha}{\alpha_c}\exp\left[\dfrac{1}{e}\dfrac{\alpha}{\alpha_c}\right], & \alpha < \alpha_c \\ \dfrac{1}{12}\alpha^2\beta J \to \infty\,, & \alpha > \alpha_c\,, \end{cases} \tag{15}$$

where $e \simeq 2.781$ is the natural number and the crossover value α_c is given by $\alpha_c = 8/e \simeq 2.943$. The effective potential height in Eq. (14) shows a discontinuity at $\alpha = \alpha_c$, beyond which it vanishes exponentially. Such an exponential decay, as well as the discontinuity, is, however, an artifact of the GTFK method since the properties of a single Josephson junction should change smoothly with α [1]. This discrepancy reflects that the essentially harmonic approximation cannot be valid for $\alpha > \alpha_c$, where the energy of the zero-point motion exceeds the bare potential height J. It is here of interest to compare the present situation with that of a double-well potential whose zero-point energy is comparable to the potential barrier [8]. In the latter case, the outer confining pontential well allows the GTFK method to work even in the presence of strong quantum fluctuations. On the other hand, for α sufficiently small compared with α_c, Eq. (14) provides us with quite a good description of the low-temperature properties.

Even though we have focused on the weak-dissipation limit ($\gamma = 0$) for simplicity, the effects of finite dissipation ($\gamma \neq 0$) can be investigated straightforwardly in the same manner. Dissipation tends to suppress quantum fluctuations, thus making the system behave more classically. For example, as shown in Fig. 2, the crossover value α_c increases with γ, and $a^2(\varphi)$ decreases rapidly with γ (notice the logarithmic scale in the plot). Similar effects are also expected in arrays, which are discussed in the following section.

III. ONE-DIMENSIONAL QUANTUM PHASE MODEL

We now turn to the QPM with many phase variables $\{\phi_j\}$, in particular, the 1D system:

$$\frac{S_0}{\hbar} = \beta J \int_0^{\beta\hbar} \frac{d\tau}{\beta\hbar} \sum_j \left[\frac{1}{2\omega_p^2} \dot{\phi}_j(\tau)^2 - \cos\varphi_j(\tau) \right], \quad (16)$$

where $\varphi_j(\tau) \equiv \phi_j(\tau) - \phi_{j+1}(\tau)$. Formally, the variational procedure is just the same as that in the previous section: We first approximate the cosine potential for every link,

$$-\cos\varphi_j(\tau) \approx \frac{\Omega_j^2(\{\varphi_{j,0}\})}{2\omega_p^2} [\varphi_j(\tau) - \varphi_{j,0}]^2 ,$$

and choose the corresponding trial action

$$\frac{S_1}{\hbar} = \frac{\beta J}{2\omega_p^2} \sum_{ij} \sum_{n=1}^{\infty} K_{n;ij} \phi_{i,n}^* \phi_{j,n}, \quad (17)$$

where the elements of the matrix K_n are given by

$$\begin{aligned} K_{n;ij} \;&=\; \omega_n^2 \delta_{ij} + [\Omega_{j-1}^2 + \Omega_j^2]\delta_{ij} \\ &\quad - \Omega_{j-1}^2 \delta_{i,j+1} - \Omega_j^2 \delta_{i,j-1}. \end{aligned} \quad (18)$$

Upon optimizing with respect to Ω_j^2, one obtains the coupled equations

$$\Omega_j^2(\{\varphi_{j,0}\}) = \omega_p^2 \exp\left[-a_j^2(\{\varphi_0\})/2\right] \cos\varphi_{j,0}, \quad (19)$$

where

$$\begin{aligned} a_j^2(\{\varphi_{j,0}\}) \equiv \frac{2\omega_p^2}{\beta J} \sum_{n=1}^{\infty} \Big[& K_{n;jj}^{-1}(\{\phi_{j,0}\}) \\ & + K_{n;j+1,j+1}^{-1}(\{\phi_{j,0}\}) - 2K_{n;j,j+1}^{-1}(\{\phi_{j,0}\}) \Big]. \end{aligned} \quad (20)$$

The effective classical Hamiltonian takes the form

$$\begin{aligned} H_{cl}(\{\varphi_j\}) \;&=\; -J \sum_j e^{-a_j^2(\{\varphi\})/2} \left[1 + a_j^2(\{\varphi\})/2\right] \cos\varphi_j \\ &\quad - \frac{1}{\beta} \sum_{n=1}^{\infty} \ln \frac{\omega_n^2}{\det K_n(\{\varphi\})}, \end{aligned} \quad (21)$$

which is again reminiscent of the usual Hamiltonian for a 1D classical JJA. The physics described by Eq. (21) is highly nontrivial, however, since the variational parameters a_j^2 and Ω_j^2 depends on the configurations of all the links of the system, not solely of their own link. To simplify the problem, KKC at this stage adopted the assumption that Ω_j^2 is constant over the whole system, independent of the configuration of the phase variables and of the link indices. This is, however, equivalent to the self-consistent harmonic approximation (SCHA) in spirit (see, *e.g.*, Ref. [12]) and may result in some mean-field character. In particular, the discontinuous change of the physical parameters at some critical value of α, which was pointed out to be an artifact of the mean-field approach, was not properly noted in KKC.

Here, we provide a slightly improved approximation, which to some restricted extent accounts for the configuration dependence of the variational parameters: $\Omega_j^2(\{\varphi_i\}) = \Omega^2(\varphi_j)$. This simplifies the expression in Eq. (20) to give

$$a^2(\varphi_j) = \frac{1}{8}\alpha^2 \beta J \{1 + F[\beta\hbar\Omega(\varphi_j)/\sqrt{2}] G[\beta\hbar\Omega(\varphi_j)/\sqrt{2}]\} \quad (22)$$

with $G(x) \equiv 2 - x\coth x$. In the low-temperature limit, the effective potential height is again given by

$$\beta\Delta U_{cl} \simeq \begin{cases} \beta J e^{-a^2(0)/2} \left[1 - \dfrac{1}{\sqrt{2}} + \dfrac{2}{e}\dfrac{\alpha}{\alpha_c}\right], & \alpha < \alpha_c \\ \beta J e^{-\alpha^2\beta J/12} \to 0, & \alpha > \alpha_c \end{cases} \quad (23)$$

with

$$a^2(0) \simeq \begin{cases} \dfrac{4}{e}\dfrac{\alpha}{\alpha_c} \exp\left[\dfrac{1}{e}\dfrac{\alpha}{\alpha_c}\right], & \alpha < \alpha_c \\ \dfrac{1}{6}\alpha^2\beta J \to \infty, & \alpha > \alpha_c . \end{cases} \quad (24)$$

In this case, the crossover value is given by $\alpha_c = 32/3\sqrt{2}e \simeq 2.775$. It appears plausible to interpret the low-temperature behavior in Eq. (23) as a remnant of the zero-temperature quantum phase transition at finite, but very low, temperatures. As already mentioned, however, this should not be taken too seriously since this behavior has its origin in an artifact arising from the GTFK variational method being applied to QPM and appears even in a (zero-dimensional) single-variable QPM. Nevertheless, for $\alpha < \alpha_c$, the GTFK variational construction in this section provides us with quite accurate physical quantities at finite temperatures.

IV. CONCLUSION

We have investigated the effects of quantum and thermal fluctuations in the 1D QPM, which may be the proper model for use with a 1D array of ultra-small Josephson-junctions, via the GTFK variational approach. The effective classical Hamiltonian, where quantum fluctuations are effectively incorporated, is derived and is shown to exhibit crossovers from classical to quantum behaviors of the fluctuations. In spite of the great success of the GTFK method for other shapes of potentials, the same method applied to the QPM has only restricted application due to the peculiar nature of the QPM.

Unlike in two dimensions, where a few experimental studies of JJAs are available, most studies in one dimension have been performed on tunnel-junction arrays with negligible Josephson coupling [13]. With the lithographic techniques already available to fabricate 2D arrays of submicron junctions with a wide range of α, it should not be difficult to perform similar experiments on 1D arrays.

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