Condensation of an Instanton Gas

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The problem of instanton interactions is considered for the case of dissipative tunneling out of a metastable state. The complex ground-state energy is expressed in terms of the pressure of the interacting instanton gas evaluated at a purely imaginary fugacity. With the Yang-Lee theory it is shown that for sufficiently small barrier height a gas-liquid condensation occurs. As a consequence the decay rate becomes much smaller than the corresponding ideal gas result. This is compared with experiments on tunneling in strongly damped superconducting quantum-interference devices.

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In many cases tunneling is a many-body problem in the sense that the considered particle couples to a large number of degrees of freedom which are not explicitly taken into account. While this applies to many microscopic problems such as the tunneling of interstitials in metals, the main recent interest in this subject did arise from the study of dissipative tunneling of the order-parameter phase in Josephson junction devices. In this context the model introduced by Caldeira and Leggett[1] has been widely used. It combines the Feynman path integral elimination of a dissipative environment and the Langer-Coleman procedure for calculating the decay rate from the imaginary part of the ground-state energy via an instanton expansion. Here we will try to investigate the limits of such an approach in cases where the barrier is no longer large compared to the zero-point energy and thus the ideal gas approximation for the instantons breaks down. This problem is of particular interest in situations with large damping where because of the strong suppression of tunneling by dissipation[1] experimental observations of the decay require small barriers. It is shown that, indeed, in this limit the instanton gas may condense into a liquid. The associated tunneling rate is much smaller than estimated from the ideal gas approximation which may explain part of the discrepancies with the Caldeira-Leggett theory found in experiments on highly damped SQUID's.[2]

We start from a path integral representation of the reduced density matrix of a single particle with coordinate q,

$$K(\tau)=\langle 0|\mathrm{Tr}_B e^{-\tau H/\hbar}|0\rangle=\int_0^0 Dq(\tau)\exp(-S/\hbar). \quad (1)$$

Its coupling to a dissipative environment is supposed to be described by a frictional force $-\eta\dot q$, which leads to an action

$$S=\int_0^\tau d\tau\left[\frac{M}{2}\dot q^2+V(q)\right]+\frac{\eta}{4\pi}\int_0^\tau\int_{-\infty}^{\infty}d\tau d\tau'\left[\frac{q(\tau)-q(\tau')}{\tau-\tau'}\right]^2. \quad (2)$$

The potential is assumed to be of the standard cubic form[1] $V=\frac{1}{2}M\omega_0^2q^2(1-q/q_0)$. From $K(\tau)$ the ground-state energy may be determined with use of the Feynman-Kac formula

$$E_0=-\lim_{\tau\to\infty}\frac{\hbar}{\tau}\ln K(\tau). \quad (3)$$

Its imaginary part—defined via an analytic continuation—then gives the decay rate of the metastable state. In the following we will *assume* that this procedure remains applicable in the presence of a dissipative environment but emphasize that a rigorous justification for this is still lacking.[3] The instanton method uses *approximate* solutions to $\delta S=0$ of the form

$$q_N(\tau)=\sum_{i=1}^N q_1(\tau-\tau_i), \quad (4)$$

where $q_1(\tau)$ is the exact single instanton solution of $\delta S=0$. Performing an appropriate analytic continuation of the formally diverging contribution from the fluctuations around q_N then gives rise to a purely imaginary contribution to $E_0=\mathrm{Re}E_0-i\hbar\Gamma/2$ and leads to a decay rate[1]

$$\Gamma_1=A\exp(-S_1/\hbar). \quad (5)$$

Here S_1 is the action of a single instanton and the prefactor A may be determined from the ratio of two determinants.[1] The real part of the energy arises from the trivial solution $q=0$ and gives the harmonic-oscillator result ($\gamma=\eta/M$)

$$\mathrm{Re}E_0=E_0^{\mathrm{osc}}=\hbar\int_0^\infty\frac{d\omega}{2\pi}\ln\left[1+\frac{\gamma}{\omega}+\frac{\omega_0^2}{\omega^2}\right]. \quad (6)$$

This expression is, in fact, divergent as $\omega\to\infty$ and becomes finite only after $1+\gamma/\omega$ is replaced by $\epsilon(i\omega)$ with ϵ the complex dielectric function.[4]

The derivation of (5) assumes widely separated instantons and approximates the action for the configuration (4) as $S_N\approx NS_1$. Quite generally the invariance of the dissipative part of the action under scale transformations $\tau\to\lambda\tau$ implies that for any extremal trajectory $\delta S=0$

the potential-energy contribution to S is equal to the kinetic energy one. This allows one to eliminate the nonlinear terms and write

$$S=\int_0^\infty \frac{d\omega}{2\pi}(2M\omega^2+\eta\omega)|q(\omega)|^2. \tag{7}$$

Here $q(\omega)$ is the Fourier transform of a general trajectory $q(\tau)$ which will always approach zero as $\tau\to\pm\infty$. Inserting (4) into (7) we obtain

$$S_N=NS_1+\hbar\sum_{i<j}\varphi(\tau_i-\tau_j), \tag{8}$$

with the second term describing the instanton interactions. The corresponding dimensionless pair potential is

$$\varphi(\tau)=\frac{2}{\hbar}\int_0^\infty \frac{d\omega}{2\pi}(2M\omega^2+\eta\omega)q_1^2(\omega)\cos\omega\tau, \tag{9}$$

where $q_1(\tau)$ and thus $q_1(\omega)$ are real and even. The interaction is repulsive for τ smaller than some τ_0 and obeys $\varphi(0)=2S_1/\hbar$. For large τ the $|\omega|$ singularity in the propagator $2M\omega^2+\eta|\omega|$ leads to an algebraically decaying attraction

$$\lim_{\tau\to\infty}\varphi(\tau)=-\frac{\eta q_1^2(\omega=0)}{\pi\hbar}\frac{1}{\tau^2}. \tag{10}$$

While attraction and repulsion have the same weight in the sense that $\int_0^\infty d\tau\varphi(\tau)=0$, in practice the repulsive part has to be replaced by a hard core in order for the instanton expansion to make sense at all.

With the inclusion of interactions the N instanton contribution to $K(\tau)$ may be written as $K_N=K_0(iy_0)^NQ_N$ with $y_0=\Gamma_1/2\omega_0$ the dimensionless single instanton decay rate and

$$Q_N(L)=\int_0^L dx_N\cdots\int_0^{x_2}dx_1\exp\left[-\sum_{i<j}\varphi(x_i-x_j)\right] \tag{11}$$

as the canonical partition function of a classical gas of N ordered particles on a line of length $L=\omega_0\tau$. Introducing the corresponding grand partition function $Y(z,L)=\sum_{N=0}^\infty z^NQ_N(L)$ for arbitrary complex z, the Feynman-Kac formula (3) takes the form

$$E_0=E_0^{\rm osc}-\hbar\omega_0 p(z=iy_0), \tag{12}$$

with $p(z)=\lim_{L\to\infty}L^{-1}\ln Y(z,L)$ the standard expression for the pressure as a function of the fugacity z. This thermodynamic formulation guarantees a proper treatment of all collective coordinates by minimizing the action with respect to the instanton separations.

Formally we have thus reduced the computation of the complex ground-state energy to the problem of determining the pressure of the classical one-dimensional instanton gas for a given complex value of the fugacity. This gas has a long-range attraction decaying as $\eta\tau^{-2}$ and thus will condense into a liquid for sufficiently large η. Nevertheless, as a result of the very small value of y_0, the ideal gas approximation may still be valid, since in the limit $z\to 0$ one expects the system to form a gas in any case. Indeed the Caldeira-Leggett[1] argument for neglecting the interactions can now be stated in the following form: By choosing the ratio $\upsilon=\Delta V/\hbar\omega_0$ sufficiently large we can always make y_0 small enough that $p(z)$ is analytic in $|z|<y_0$. Thus the Mayer virial expansion $p(z)=\sum_{l=1}^\infty b_lz^l$ converges at $z=iy_0$ with $b_1=1$, $b_2=\int_0^\infty dx(e^{-\varphi(x)}-1)$, etc. The corresponding results $\Gamma=\Gamma_1(1-b_3y_0^2+\cdots)$ and $\mathrm{Re}E_0=E_0^{\rm osc}+\hbar\omega_0b_2y_0^2$ then give corrections to the ideal gas expressions [(5) and (6)] which can be made arbitrarily small. In the following we will argue that while this assertion is formally correct, in practice one is often interested in small υ which is true in particular in cases where the dimensionless damping $\alpha=\gamma/2\omega_0$ is large compared to one. In such a situation we will find that below a certain $\bar\upsilon(\alpha)$ the gas condenses even if y_0 is extremely small and the condition $S_1/\hbar\gg 1$ is *not* sufficient to guarantee the validity of the ideal gas approximation.

To obtain a precise criterion for the radius of convergence of the virial expansion we will confine our attention to the regime $\alpha\gg 1$ and then use a lattice gas picture. For large α the single instanton solution may be obtained analytically as [1]

$$q_1(\omega)=\tfrac{4}{3}\pi q_0\tau_c\exp(-|\omega|\tau_c), \tag{13}$$

with $\tau_c=\gamma/\omega_0^2$. The corresponding instanton interaction is

$$\varphi(x)=12\pi\alpha\upsilon\frac{1-(x/x_0)^2}{[1+(x/x_0)^2]^2}, \tag{14}$$

with $x=\omega_0\tau$, $x_0=4\alpha$, and $12\pi\alpha\upsilon$ as the large damping value of $2S_1/\hbar$. The corrections to (14) are of order α^{-2} and thus are negligible if $\alpha\gg 1$. We now approximate the continuum by a lattice gas, replacing the repulsive interaction for $x<x_0$ by a hard core and introducing occupation numbers $n_i=0,1$ for a discrete set of points $x_i=ix_0$. Then

$$\sum_{i<j}\varphi(x_i-x_j)\to -\sum_{l=1}^\infty \epsilon_l\sum_{i=1}^{N_0}n_in_{i+l}, \tag{15}$$

with

$$\epsilon_l=-\varphi(lx_0)=12\pi\alpha\upsilon\frac{l^2-1}{(l^2+1)^2} \tag{16}$$

and $N_0=L/x_0$ the number of sites. According to the theory of Yang and Lee[5] the corresponding grand partition function is then a polynomial of degree N_0 which has all its zeros on $|z|=R=e^{-\sigma}$ where

$$\sigma=\sum_{l=1}^\infty\epsilon_l \underset{\alpha\gg1}{\longrightarrow} 6\pi\alpha\upsilon[1-(\pi/\sinh\pi)^2]. \tag{17}$$

In the thermodynamic limit $N_0\to\infty$ the pressure is an analytic function of z both inside and outside $|z|=R$ and may be expressed as

$$p(z)=\int_0^\pi d\Theta g(\Theta)\ln\left[1-2\frac{z}{R}\cos\Theta+\left(\frac{z}{R}\right)^2\right], \tag{18}$$

where $g(\Theta)=g(-\Theta)$ is the density of Yang-Lee zeros on the circle $|z|=R$, normalized according to $\int_0^\pi d\Theta g(\Theta)=\frac{1}{2}$. It is determined by the cluster integrals b_l via

$$g(\Theta)=\frac{1}{2\pi}-\frac{1}{\pi}\sum_{l=1}^{\infty} lR^l b_l \cos l\Theta. \tag{19}$$

As is explained by Yang and Lee[5] the general behavior of $g(\Theta)$ for a system exhibiting condensation is such that for small coupling $g(\Theta)$ is concentrated on $\Theta_L \le \Theta \le \pi$. With increasing σ the Yang-Lee angle Θ_L decreases and approaches zero at the critical point $\sigma=\sigma_c$ where $p(z)$ becomes nonanalytic along the real positive z axis. If σ increased further, $g(\Theta)$ is distributed more uniformly on the circle whose radius R rapidly goes to zero. It is this latter regime which will be of interest to us and where, in fact, our lattice gas approximation should be rather accurate.[6] In order to estimate the critical point we approximate (16) by a pure l^{-2} term plus a nearest-neighbor contribution which makes $\epsilon_1=0$, i.e., we take $\epsilon_l \approx \epsilon_{\mathrm{LR}}/l^2$ for $l\ge 2$ with $\epsilon_{\mathrm{LR}}=12\pi\alpha\upsilon$. The equation determining the critical value of ϵ_{LR} can then be taken from Anderson and Yuval[7] to be

$$\epsilon_{\mathrm{LR}}^c=2+4\exp(-C\epsilon_{\mathrm{LR}}^c/2), \tag{20}$$

with $C=0.577\ldots$ being Euler's constant. Its solution is $\epsilon_{\mathrm{LR}}^c \approx 3.47$, and thus whenever $\alpha\upsilon>(\alpha\upsilon)^c\approx 0.1$ (Ref. 8) we are below the critical point for condensation. As emphasized above, however, the instanton gas will actually be in the liquid phase at a fugacity $|z|=y_0$ only if $y_0 \ge R$. Now the critical fugacity $z_c=e^{-\sigma_c}$ is $z_c=0.107$ in the approximation of a pure l^{-2} interaction for $l\ge 2$ and thus is large compared to any reasonable value of y_0. However, the strong decrease of R with increasing coupling makes it possible to fulfill the condition for condensation $y_0=R$ in a certain range of the parameters α and υ. Writing $A/2\omega_0=\sqrt{\upsilon}c(\alpha)$ with a function $c(\alpha)$ which approaches $4\sqrt{6}\alpha^{7/2}$ for $\alpha\gg 1$,[9] the condition for a liquid-gas condensation at $|z|=y_0$ may be written as

$$\ln[\sqrt{\upsilon}c(\alpha)]=S_1/\hbar-\sigma \underset{\alpha\gg 1}{\longrightarrow} 6\pi\alpha\upsilon(\pi/\sinh\pi)^2. \tag{21}$$

This equation may be solved graphically, and in the considered range $\alpha\gg 1$ its solution is given rather accurately by

$$\bar{\upsilon}(\alpha) \underset{\alpha\gg 1}{\approx} \frac{\ln c(\alpha)}{6\pi\alpha(\pi/\sinh\pi)^2}. \tag{22}$$

The corresponding phase boundary is shown in Fig. 1 where the expected behavior for smaller α follows from the fact that $S_1/\hbar-\sigma$ should approach a constant larger than $\ln[\sqrt{\upsilon}c(0)]$. Since $\ln c(\alpha)$ is concave, the existence of a solution of (21) for large α necessarily implies that of a second one at lower α. We have therefore found that for small enough υ—but still in the range $S_1/\hbar\gg 1$—the instanton gas condenses into a liquid and thus the ideal gas picture will certainly break down.

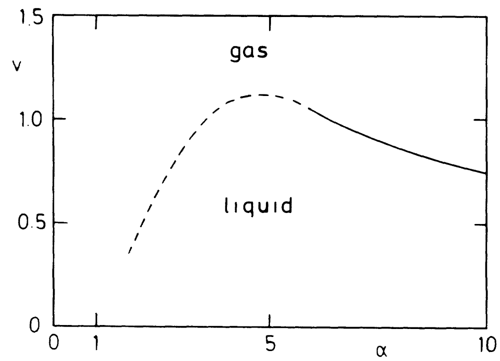

FIG. 1. The gas-liquid phase boundary in the υ,α plane. The full line represents the result (22) valid for strong damping $\alpha\gg 1$, while the dotted line indicates *qualitatively* the expected behavior at smaller α.

This raises the question whether the instanton approach may be extended into the liquid phase. Within our statistical mechanics analogy this is indeed possible. As pointed out by Yang and Lee, $p(z)$ may be interpreted as the complex logarithmic potential of an infinite charged cylinder with line charge density $g(\Theta)$.[5] Since $\mathrm{Re}p=\mathrm{const}$ are the equipotential lines, the real part of the energy is continuous across $|z|=R$. Problems, however, arise in the decay rate since $\mathrm{Im}p=\mathrm{const}$ gives the corresponding lines of force which are discontinuous across the charged circle. Indeed, the associated electric field $E^*=2p'(z)=E_x-iE_y$ makes a jump of magnitude $2\pi g(\Theta)$ at $z=Re^{i\Theta}$. Using the Cauchy-Riemann conditions, this implies that both $R\partial_r \mathrm{Re}p$ and $\partial_\Theta \mathrm{Im}p$ jump by $2\pi g(\Theta)$ in crossing the phase boundary. Thus in a case where $g(\Theta)$ is distributed over the whole circle (i.e., for $\alpha\upsilon>0.1$) $\mathrm{Im}p$ can be continuous only at a single point on $|z|=R$. In addition Gauss's law for the enclosed charge shows that $\mathrm{Im}p$ is multivalued for $|z|>R$, increasing by 2π for each winding around $z=0$. In order to extend the instanton expansion into the liquid regime in a meaningful way, we require $\mathrm{Im}p$ to be continuous across $z=iR$ which is achieved by integrating the continuous function $\partial_y \mathrm{Im}p(z=iy)$ across the boundary. Since we are interested in the regime much below the critical point, the expansion (19) will converge uniformly on the circle and thus in the limit $R\to 0$ only the universal $l=1$ term correction to the uniform distribution needs to be taken into account. With this approximation, which neglects the corrections to the ideal gas results *inside* $|z|=R$ we finally obtain

$$\mathrm{Re}p(z=iy)=\begin{cases}0, & \text{for } y<R,\\ \ln y/R, & \text{for } y>R,\end{cases} \tag{23}$$

and

$$\mathrm{Im}p(z=iy)=\begin{cases}y, & \text{for } y<R,\\ 2R-R^2/y, & \text{for } y>R.\end{cases} \tag{24}$$

Thus in the liquid regime $v < \bar{v}(\alpha)$ the real part of the energy is reduced compared to $E_0^{\rm osc}$ by an amount $-\hbar\omega_0 \ln y_0/R$. At the same time the decay rate $\Gamma = 2\omega_0 \mathrm{Im} p(z = iy_0)$ is smaller than its ideal gas value $\Gamma_1 = 2\omega_0 y_0$ valid for $y_0 < R$. In the limit $y_0 \gg R$ it approaches a value $4\omega_0 R$ which is completely determined by the instanton interactions. The precise numerical value of R depends on the interaction potential also on short distances and on the way the lattice gas transcription is performed.[10] Therefore the phase diagram shown in Fig. 1 is valid only approximately.

Our results indicate that for the measurements on highly damped SQUID's[2] which have explored the regime $\alpha \approx 4$ and $v \simeq 0.5$ the instantons should already be condensed. In fact it was found[2] that the observed rate was much smaller than predicted, in agreement with the present results. As an estimate we use $\Gamma_1/\Gamma \approx y_0/2R$ for $R \ll y_0$, which is approximately equal to $(\bar{v})^{1/2} c(\alpha)/2$ since σ is close to $S_1/\hbar$. Thus for the relevant parameters the Caldeira-Leggett theory will overestimate the rate by about 3 orders of magnitude, the discrepancy being essentially due to the prefactor. While this would explain at least part of the disagreement found in Ref. 2, it has been claimed recently[11] that the original estimate of the barrier height was too small and indeed the results could be understood on the basis of the standard theory. Regarding, however, that at $\alpha \gg 1$ the rate is extremely sensitive to even tiny changes in v, it seems that with present uncertainties in the parameter values it is hard to draw definite conclusions. In addition we believe that, independent of a possible previous experimental evidence, the possibility of a qualitative breakdown of the dilute instanton approximation is interesting in itself and should be observable in further careful measurements along the lines in Ref. 2.

Finally, it should be mentioned that instanton interactions have previously been discussed—for vanishing dissipation—in the degenerate quartic double well within a very different treatment.[12] Indeed, the attractive long distance interaction there was used at *all* distances, thereby requiring analytic continuation to prevent instability. By contrast, the instanton interactions in the present, quite different, problem were shown to be repulsive at short distances and replacing them by a hard core leads both to well defined instantons and proper thermodynamics.

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[1]A. O. Caldeira and A. J. Leggett, Ann. Phys. (N.Y.) **149**, 374 (1984), and **153**, 445(E) (1984).

[2]D. B. Schwartz, B. Sen, C. N. Archie, and J. E. Lukens, Phys. Rev. Lett. **55**, 1547 (1985).

[3]A. Schmid, Ann. Phys. (N.Y.) **170**, 333 (1986). This work indicates that a WKB derivation of the instanton result runs into difficulties if the environment spectrum is gapless, and applies to our case.

[4]W. Zwerger, Z. Phys. B **47**, 129 (1982).

[5]C. N. Yang and T. D. Lee, Phys. Rev. **87**, 404 (1952); T. D. Lee and C. N. Yang, Phys. Rev. **87**, 410 (1952).

[6]Indeed in a one-dimensional van der Waals gas far below its critical point the Yang-Lee zero distribution is essentially identical to that of a lattice gas; see P. C. Hemmer and E. H. Hauge, Phys. Rev. **133**, A 1010 (1964).

[7]P. W. Anderson and G. Yuval, J. Phys. C **4**, 607 (1971).

[8]By considering the general asymptotic behavior (10) of $\varphi(\tau)$, it is possible to show that this estimate remains valid for *all* α.

[9]H. Grabert, P. Olschowski, and U. Weiss, Phys. Rev. B **36**, 1931 (1987).

[10]This is in contrast to the localization in a dissipative double-well potential discussed by S. Chakravarty, Phys. Rev. Lett. **49**, 681 (1982); A. J. Bray and M. A. Moore, Phys. Rev. Lett. **49**, 1546 (1982).

[11]A. D. Zaikin and S. V. Panyukov, Pis'ma Zh. Eksp. Teor. Fiz. **43**, 518 (1986) [JETP Lett. **43**, 670 (1986)].

[12]J. Zinn-Justin, Nucl. Phys. **B218**, 333 (1983).