Regularization and Counterterms in Quantum Mechanics

Adam Ball

Regularization and counterterms are some of the most elusive aspects of quantum field theory (QFT), but they already show up in the quantum mechanics (QM) path integral and much can be gained from studying them there. In particular, one-dimensional (1D) QM can be viewed as 1D scalar QFT and so in that case the lessons carry over directly. In this note we compute the 1D QM partition function in several different ways, in the process gaining insight into regularization and counterterms.

Particle on a circle

Consider the QM of a free particle on a circle of radius R, i.e. $x \sim x + 2\pi R$. The Hamiltonian is

$$H = \frac{p^2}{2m} \tag{1}$$

and the Lagrangian is

$$L = \frac{1}{2} m \dot{x}^2 \tag{2}$$

The position and momentum are classically related as $p = m\dot{x}$, where a dot indicates a time derivative. I set $c = \hbar = 1$ but keep other units around. I will keep track of the mass dimension, e.g. $1 = [m] = [p] = -[x] = -[t] = -[R]$. The quantum momentum is quantized due to the periodicity of x. I will not go into detail here, but an easy way to remember the quantization condition is that $p \sim -i\partial_x$ (following from $[x, p] = i$) and single-valued wavefunctions are like $e^{inx/R}$ with $n \in \mathbb{Z}$, and therefore $p = n/R$. The partition function at inverse temperature β is defined as a canonical trace, and we can easily evaluate it in the orthonormal momentum basis $\langle\, m \mid n \,\rangle = \delta_{mn}$,

$$\begin{aligned} Z(\beta) &= \operatorname{Tr} e^{-\beta H} \\ &= \sum_n \langle\, n \,| e^{-\beta H} |\, n \,\rangle \\ &= \sum_n \exp\left[-\frac{\beta n^2}{2mR^2}\right] \\ &= \vartheta_3(e^{-\beta/2mR^2}) \end{aligned} \tag{3}$$

where $\vartheta_3(q)$ is EllipticTheta[3,0,q] in Mathematica. In the $R \to \infty$ limit the leading term is

$$Z(\beta) \overset{R\to\infty}{\longrightarrow} 2\pi R \sqrt{\frac{m}{2\pi\beta}} \tag{4}$$

We see that it diverges, but this is expected for an extensive thermodynamic quantity. We will keep the divergent volume factor $2\pi R$ explicit; one can view R as an infrared (IR) regulator for the divergent partition function of a particle on an infinite line. In contrast, the path integral subtleties that are the main focus of this note have more to do with ultraviolet (UV) divergences. Before moving on, we note that the partition function is written as a function of β, but by dimensional analysis it can only involve dimensionless combinations of the dimensionful parameters in play: R, m, β. The particular dimensionless combination mR^2/β turns out to be the only one used. If we rescaled all physical scales by a common factor, i.e. $R, m, \beta \to \lambda R, \lambda^{-1} m, \lambda\beta$, then the partition function (and all physics, really) would be unchanged.

In summary, this note is about computing the QM partition function of a particle on an infinite line, IR-regulated as a very large circle, in several different ways.[1] We have just seen that the canonical trace method gives

$$\boxed{Z_{\text{canon}}(\beta) = 2\pi R\sqrt{\frac{m}{2\pi\beta}}} \tag{5}$$

Lattice

Next let's compute the partition function by discretizing time (but not space). This is basically how the path integral is often introduced in QM textbooks. See for example Shankar 21.1.16-17. However we will not derive the precise discretized measure and action, instead *defining* them somewhat arbitrarily as regularizations of the continuum theory and allowing for an overall energy counterterm E_0 that can depend on the UV cutoff and the system's parameters R, m but not on the temperature β, which is independent from the system itself. We break the thermal circle into N intervals of size $\Delta = \beta/N$. Here Δ is viewed as the independent variable, not N. We define the regularized action

$$S_{\text{reg}} = \beta E_0 + \frac{1}{2}m\Delta\sum_{i=1}^{\beta/\Delta}\left(\frac{x_i - x_{i-1}}{\Delta}\right)^2 \tag{6}$$

In anticipation of the regularization being "not quite right" we have allowed for an arbitrary energy counterterm E_0 in the Lagrangian. This turns out to be the only one we need. We define the regularized path integral measure

$$(\mathcal{D}x)_{\text{reg}} = \prod_{i=1}^{\beta/\Delta}\frac{dx_i}{\Delta} \tag{7}$$

The path integral measure must be dimensionless, and we achieved this rather arbitrarily with powers of the UV cutoff Δ; any factor independent of β would have sufficed. The regularized partition function reduces to coupled Gaussian integrals and can be evaluated exactly (up to terms exponentially suppressed by R), yielding

$$\begin{aligned}\int\left(\prod_{i=1}^{\beta/\Delta}\frac{dx_i}{\Delta}\right)\exp\left[-\beta E_0 - \frac{1}{2}m\Delta\sum_{i=1}^{\beta/\Delta}\left(\frac{x_i - x_{i-1}}{\Delta}\right)^2\right] &= \frac{2\pi R\, e^{-\beta E_0}}{\Delta\sqrt{\beta/\Delta}}\left(\frac{2\pi}{m\Delta}\right)^{\frac{\beta}{2\Delta}-\frac{1}{2}} \\ &= \frac{2\pi R}{\sqrt{2\pi\beta/m}}\exp\left[-\beta E_0 + \frac{\beta}{2\Delta}\log\frac{2\pi}{m\Delta}\right]\end{aligned} \tag{8}$$

We see that choosing

$$E_0 = \frac{1}{2\Delta}\log\frac{2\pi}{m\Delta} + E_{\text{ren}} \tag{9}$$

where the "renormalized" energy E_{ren} is independent of R, m, β, and Δ. It yields a partition function independent of Δ, and we can safely take the $\Delta \to 0$ limit to get

$$\boxed{Z_{\text{lattice}}(\beta) = 2\pi R\sqrt{\frac{m}{2\pi\beta}}\,e^{-\beta E_{\text{ren}}}} \tag{10}$$

This agrees with Z_{canon} up to the overall energy shift by E_{ren}, and one might argue that this can only be determined by measurement in the first place anyway so we're not really losing any information at all.

[1] For finite R the path integral must take winding modes into account, but they are exponentially suppressed by R and so can be ignored in our large-R context.

Fourier

Next use Fourier regularization. We expand $x(t)$ in orthonormal Fourier modes and impose a momentum cutoff Λ. Let $N = \Lambda\beta$ be the number of modes we end up keeping, and for simplicity assume N is odd. One should think of Λ as the independent parameter, not N. We have

$$x(t) = \frac{a_0}{\sqrt{\beta}} + \sqrt{\frac{2}{\beta}} \sum_{n=1}^{\frac{N-1}{2}} \left(a_n \cos \frac{2\pi n t}{\beta} + b_n \sin \frac{2\pi n t}{\beta} \right) \tag{11}$$

Note the periodicity of x means $a_0 \sim a_0 + 2\pi R\sqrt{\beta}$. The normalization is such that

$$\int_0^\beta dt\, x(t)^2 = \beta \left(\frac{a_0^2}{\beta} + \frac{2}{\beta} \sum_{n=1}^{\frac{N-1}{2}} \left(\frac{1}{2} a_n^2 + \frac{1}{2} b_n^2 \right) \right) = a_0^2 + a_1^2 + \ldots \tag{12}$$

We adopt the measure

$$(\mathcal{D}x)_{\text{reg}} = \Lambda^{3/2} da_0 \prod_{n=1}^{\frac{N-1}{2}} \Lambda^3 da_n db_n \tag{13}$$

where once again we used powers of the cutoff to make the measure dimensionless. The action in these variables is

$$S[x] = \beta E_0 + \frac{m}{2} \sum_{n=1}^{\frac{N-1}{2}} \left(\frac{2\pi n}{\beta} \right)^2 (a_n^2 + b_n^2) \tag{14}$$

The partition function contribution from a_n is

$$\int \Lambda^{3/2} da_n \, \exp\left[-\frac{m}{2} \left(\frac{2\pi n}{\beta} \right)^2 a_n^2 \right] = \frac{\Lambda^{3/2}\beta}{n\sqrt{2\pi m}} = \frac{N^{3/2}}{n\sqrt{2\pi m \beta}} \tag{15}$$

The full partition function is then

$$\begin{aligned} Z_{\text{Fourier}}(\beta) &= \Lambda^{3/2} 2\pi R \sqrt{\beta} \prod_{n=1}^{\frac{N-1}{2}} \left(\frac{N^{3/2}}{n\sqrt{2\pi m\beta}} \right)^2 e^{-\beta E_0} \\ &= \frac{2\pi R\, N^{3/2}}{\beta} \left(\frac{N^{3/2}}{\sqrt{2\pi m \beta}} \right)^{N-1} \left(\frac{N-1}{2} \right)!^{-2} e^{-\beta E_0} \end{aligned} \tag{16}$$

The Stirling approximation states

$$\left(\frac{N-1}{2} \right)! \approx \sqrt{2\pi \frac{N-1}{2}} \left(\frac{N-1}{2e} \right)^{\frac{N-1}{2}} \tag{17}$$

and therefore at leading order we have

$$\begin{aligned} Z_{\text{Fourier}}(\beta) &= \frac{2\pi R\, N^{3/2}}{\beta} \left(\frac{N^{3/2}}{\sqrt{2\pi m\beta}} \right)^{N-1} \frac{1}{\pi(N-1)} \left(\frac{2e}{N-1} \right)^{N-1} e^{-\beta E_0} \\ &= \frac{2\pi R N^{1/2}}{\pi\beta} \left(\frac{N^{1/2}}{\sqrt{2\pi m\beta}} \right)^{N-1} \left(1 - \frac{1}{N} \right)^{-N} (2e)^{N-1} e^{-\beta E_0} \\ &= \frac{2\pi R N^{1/2}}{2\pi\beta} \left(\frac{N^{1/2}}{\sqrt{2\pi m\beta}} \right)^{N-1} (2e)^N e^{-\beta E_0} \\ &= 2\pi R \sqrt{\frac{m}{2\pi\beta}} \left(\frac{4e^2\Lambda}{2\pi m} \right)^{N/2} e^{-\beta E_0} \\ &= 2\pi R \sqrt{\frac{m}{2\pi\beta}} \exp\left[-\beta E_0 + \frac{1}{2} \beta\Lambda \log \frac{4e^2\Lambda}{2\pi m} \right] \end{aligned} \tag{18}$$

We see that choosing

$$E_0 = \frac{1}{2}\Lambda \log \frac{4e^2\Lambda}{2\pi m} + E_{\text{ren}} \tag{19}$$

results in

$$\boxed{Z_{\text{Fourier}}(\beta) = 2\pi R\sqrt{\frac{m}{2\pi\beta}}\, e^{-\beta E_{\text{ren}}}} \tag{20}$$

This is the exact same result as for the lattice regularization.

Zeta function

Finally let's try zeta regularization. Once again we expand in orthonormal Fourier modes, but this time we keep the whole infinite series,

$$x(t) = \frac{a_0}{\sqrt{\beta}} + \sqrt{\frac{2}{\beta}}\sum_{n=1}^{\infty}\left(a_n \cos\frac{2\pi n t}{\beta} + b_n \sin\frac{2\pi n t}{\beta}\right) \tag{21}$$

For the measure we take

$$(\mathcal{D}x)_{\text{reg}} = \Lambda^{3/2} a_0 \prod_{n=1}^{\infty} \Lambda^3 da_n db_n \tag{22}$$

where now Λ is an arbitrary mass scale (independent of R, m, β) inserted to keep the measure dimensionless. It is not necessarily large. Proceeding with the path integral, we get a zero mode factor and a functional determinant

$$\begin{aligned} Z_{\text{zeta}}(\beta) &= \Lambda^{3/2} 2\pi R\sqrt{\beta}\, \det{}'\big(\frac{m}{2\pi\Lambda^3}\partial_t^2\big)^{-1/2} \\ &= \Lambda^{3/2} 2\pi R\sqrt{\beta} \prod_{n=1}^{\infty}\left(\frac{\Lambda^{3/2}\beta}{n\sqrt{2\pi m}}\right)^2 \end{aligned} \tag{23}$$

The prime in $\det'$ indicates that we omit the zero mode in computing the determinant. The infinite product can be evaluated with zeta function regularization. Given an operator D with spectrum λ_n (with any zero modes omitted), one defines the zeta function

$$\zeta_D(s) \equiv \sum_n \lambda_n^{-s} \tag{24}$$

Then formally

$$\zeta_D'(s) = -\sum_n \lambda_n^{-s} \log \lambda_n \tag{25}$$

and so

$$e^{-\zeta_D'(0)} = \prod_n \lambda_n = \det D \tag{26}$$

Performing these manipulations here gives

$$Z_{\text{zeta}}(\beta) = \Lambda^{3/2} 2\pi R\sqrt{\beta}\frac{\sqrt{2\pi m}}{2\pi\Lambda^{3/2}\beta} \tag{27}$$

Simplifying slightly, the final form is

$$\boxed{Z_{\text{zeta}}(\beta) = 2\pi R\sqrt{\frac{m}{2\pi\beta}}} \tag{28}$$

We have another match. Note that Λ dropped out on its own, with no need for a counterterm.