

Path-Integral Approach to a Quantum Particle in Random Potential with Long-Range Correlations

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ABSTRACT

The mean square displacement of a quantum particle in random potential with long-range correlations is computed exactly using the path-integral method. The result agrees with the replica method while the variation of the mean square displacement with the density of disorder is found in our approach.

Key words: path-integral, random potential, disordered system

INTRODUCTION

There has been much interest in the problem of a quantum particle in random potential. Since this problem is directly related to diverse fields of disordered systems such as the behavior of polymers in random media (Kunsombat and Sa-yakanit, 2004 and 2005), the behavior of flux lines in superconductors in the presence of columnar defects (Nelson and Vinokur, 1993; Goldschmidt, 1997), the problem of diffusion in a random catalytic environment (Nattermann and Renz, 1989) and the behavior of an electron in a dirty metal. Despite the volume of work has been done on these problems, there are still many unanswered questions. In general, the random system has very complicated structures. In order to understand these complex problems, several researchers usually modeled the disorder with short-range or long-range correlations and then calculated the mean square displacement using the replica method (Edwards and Muthukumar, 1988; Goldschmidt and Blum, 1993; Goldschmidt, 2000; Shiferaw and Goldschmidt, 2000).

Recently, Shiferaw and Goldschmidt (2000) considered a model of a quantum particle in random potential with long-range quadratic correlations. They also used the replica method to calculate exactly the mean square displacement of a quantum particle. The result was

$$\langle \bar{X}^2 \rangle = \frac{2dg}{\mu^{2\xi^2}} + \frac{d\hbar}{2\sqrt{\mu m}} \coth \left(\frac{\beta \hbar}{2} \sqrt{\frac{\mu}{m}} \right). \quad (1)$$

Where d is the dimensions of the system, g is the strength of disorder, ξ is the correlation length, μ is the strength of the harmonic potential, \hbar is Planck's constant, m is the mass of a particle and $\beta = 1/k_B T$, where k_B is Boltzmann's constant and T is the absolute temperature. The result shown above agreed with an alternative numerical solution and was valid in case of very long-range correlations.

Although the replica method is one of the most powerful theoretical tools, the calculation in this method is very difficult. When the result of this calculation does not work, the symmetry of the replica will be broken. The new calculation must be done. This always leads to more complicated calculations. In this paper, we derive the exact analytical result, using only the path-integral method without the replica.

MATERIALS AND METHODS

We first consider a particle moving in a set of N rigid scatterers, confined within a volume Ω , and having a density $\rho = N/\Omega$. The propagator of such a system can be expressed in the path-integral representation as

$$G(\vec{X}_2, \vec{X}_1; t) = \int_{\vec{X}_1}^{\vec{X}_2} D[\vec{X}(\tau)] \times \exp \left\{ \frac{i}{\hbar} \int_0^t d\tau \left(\frac{m}{2} \dot{\vec{X}}^2(\tau) - \frac{\mu}{2} \vec{X}^2(\tau) \right) + \sum_{i=1}^N \int_0^t d\tau v[\vec{X}(\tau) - \vec{R}_i] \right\}. \quad (2)$$

Eq. (2) denotes the path integral that goes from $\vec{X}(0) = \vec{X}_1$ to $\vec{X}(t) = \vec{X}_2$. Where $\vec{X}(\tau)$ is the d -dimensional position vector of a particle at time τ , $v[\vec{X}(\tau) - \vec{R}_i]$ represents the potential of a single scatterer at \vec{R}_i . The harmonic term is included to mimic the effects of finite volume, where μ is the strength of the harmonic potential and defines the system size, μ approach zero in the infinite volume limit.

Next, we assume that the obstacles are randomly distributed throughout the volume Ω of the medium with a random distribution

$$P[\vec{R}] d([\vec{R}]) = \prod_{i=1}^N \left(\frac{d\vec{R}_i}{\Omega} \right). \quad (3)$$

The average over all configurations of the random obstacles of Eq. (2) can be performed exactly (Sayanit, 1974). This yields in the limit $N \rightarrow \infty$ and $\Omega \rightarrow \infty$. The result may be obtained as

$$\begin{aligned} \bar{G}(\vec{X}_2, \vec{X}_1; t) &= \int G(\vec{X}_2, \vec{X}_1; t) P[\vec{R}] d([\vec{R}]) \\ &= \int D[\vec{X}(\tau)] \exp \left\{ \frac{i}{\hbar} \int_0^t d\tau \left(\frac{m}{2} \dot{\vec{X}}^2(\tau) - \frac{\mu}{2} \vec{X}^2(\tau) \right) \right. \\ &\quad \left. + \rho \int d\vec{R} \left[\exp \left(\frac{-i}{\hbar} \int_0^t v[\vec{X}(\tau) - \vec{R}] d\tau \right) - 1 \right] \right\}. \end{aligned} \quad (4)$$

In the limits of high density $\rho \rightarrow \infty$ and weak scattering potential $v \rightarrow 0$, so that ρv^2 remains finite, Eq. (4) can be simplified and rewritten in the form

$$\bar{G}(\vec{X}_2, \vec{X}_1; t) = \int_{\vec{X}_1}^{\vec{X}_2} D[\vec{X}(\tau)]$$

$$\times \exp \left\{ \frac{i}{\hbar} \left[\int_0^t d\tau \left(\frac{m}{2} \dot{\bar{X}}^2(\tau) - \frac{\mu}{2} \bar{X}^2(\tau) \right) + \frac{i\rho\eta^2}{2\hbar} \int_0^t \int_0^t d\tau d\sigma W[\bar{X}(\tau) - \bar{X}(\sigma)] \right] \right\} \quad (5)$$

Here, the mean potential energy has been taken as zero. The η is a parameter, it is explicitly writing here in order to take care the dimension of the system and $W[\bar{X}(\tau) - \bar{X}(\sigma)]$ denotes the correlation function, defined as

$$W[\bar{X}(\tau) - \bar{X}(\sigma)] = \int v[\bar{X}(\tau) - \bar{R}] v[\bar{X}(\sigma) - \bar{R}] d\bar{R}. \quad (6)$$

In order to compare our result with the replica method, we use the model of Shiferaw and Goldschmidt (2000). It is given by

$$W[\bar{X}(\tau) - \bar{X}(\sigma)] = g \left(1 - \frac{(\bar{X}(\tau) - \bar{X}(\sigma))^2}{\xi^2} \right). \quad (7)$$

Where in this model, ξ is chosen to be larger than the medium size, so that the correlation function is well defined (non-negative) over the entire medium. Substituting Eq. (7) into Eq. (5), the average propagator becomes

$$\begin{aligned} \bar{G}(\bar{X}_2, \bar{X}_1; t) &= \int_{\bar{X}_1}^{\bar{X}_2} D[\bar{X}(\tau)] \\ &\times \exp \left(\frac{i}{\hbar} \left[\int_0^t d\tau \left(\frac{m}{2} \dot{\bar{X}}^2(\tau) - \frac{m\omega^2}{2} \bar{X}^2(\tau) \right) + \frac{i\rho\eta^2 g}{\hbar \xi^2} \int_0^t \int_0^t d\tau d\sigma \bar{X}(\tau) \cdot \bar{X}(\sigma) \right] \right). \end{aligned} \quad (8)$$

Where $\omega = \left(\frac{2i\rho\eta^2 g t}{m\hbar \xi^2} + \frac{\mu}{m} \right)^{1/2}$ and where we have dropped the constant part of the action, since it only contributes an unimportant normalization factor. Eq. (8) can be evaluated by using Stratonovich's transformation (Sa-yakanit *et al.*, 1988) with respect to the Gaussian distribution of the constant force \vec{F} . We will call the result the effective system. The relation between the average propagator and the effective propagator can be written in the form

$$\bar{G}(\bar{X}_2, \bar{X}_1; t) = \left\langle G_{eff}(\bar{X}_2, \bar{X}_1; t) \right\rangle_{\vec{F}}. \quad (9)$$

The symbol $\langle O \rangle_{\vec{F}}$ denotes the Gaussian average defined by

$$\langle O \rangle_{\vec{F}} = \frac{\int_{-\infty}^{+\infty} O \exp \left(-\frac{\xi^2}{4\rho\eta^2 g} \vec{F}^2 \right) d\vec{F}}{\int_{-\infty}^{+\infty} \exp \left(-\frac{\xi^2}{4\rho\eta^2 g} \vec{F}^2 \right) d\vec{F}}. \quad (10)$$

The effective propagator $G_{eff}(\bar{X}_2, \bar{X}_1; t)$ is corresponding to the system of a particle moving in the forced harmonic oscillator, which can be directly evaluated (Feynman and Hibbs, 1995), and given by

$$G_{eff}(\bar{X}_2, \bar{X}_1; t) = \left(\frac{m\omega}{2\pi i\hbar \sin \omega t} \right)^{d/2}$$

$$\begin{aligned} & \times \exp \left[\frac{i}{\hbar} \left\{ -\frac{m\omega}{4} \tan\left(\frac{\omega t}{2}\right) (\vec{X}_2 + \vec{X}_1)^2 + \frac{m\omega}{4} \cot\left(\frac{\omega t}{2}\right) (\vec{X}_2 - \vec{X}_1)^2 \right. \right. \\ & \left. \left. + \frac{\vec{F}}{\omega} \tan\left(\frac{\omega t}{2}\right) (\vec{X}_2 + \vec{X}_1) - \frac{\vec{F}^2}{m\omega^3} \left(\tan\left(\frac{\omega t}{2}\right) - \frac{\omega t}{2} \right) \right\} \right]. \end{aligned} \quad (11)$$

By applying Eq. (9) to Eq. (11), we obtain

$$\begin{aligned} \bar{G}(\vec{X}_2, \vec{X}_1; t) = & \left(\frac{\xi^2}{4\rho\eta^2 g} \right)^{d/2} \left(\frac{m\omega}{2\pi i\hbar \sin \omega t} \right)^{d/2} \left(\frac{\pi}{\frac{\xi^2}{4\rho\eta^2 g} + \frac{i \tan \frac{\omega t}{2}}{\hbar m\omega^3} - \frac{i\omega t}{2\hbar m\omega^3}} \right)^{d/2} \\ & \times \exp \left[-\frac{(\vec{X}_2 + \vec{X}_1)^2 \tan^2\left(\frac{\omega t}{2}\right)}{4\hbar^2 \omega^2 \left(\frac{\xi^2}{4\rho\eta^2 g} + \frac{i \tan \frac{\omega t}{2}}{\hbar m\omega^3} - \frac{i\omega t}{2\hbar m\omega^3} \right)} \right. \\ & \left. - \frac{i m\omega}{4\hbar} \tan\left(\frac{\omega t}{2}\right) (\vec{X}_2 + \vec{X}_1)^2 + \frac{i m\omega}{4\hbar} \cot\left(\frac{\omega t}{2}\right) (\vec{X}_2 - \vec{X}_1)^2 \right]. \end{aligned} \quad (12)$$

The mean square displacement of a particle can be evaluated by the expression

$$\langle \vec{X}^2 \rangle = \frac{\int \vec{X}^2 \rho(\vec{X}, \vec{X}) d\vec{X}}{\int \rho(\vec{X}, \vec{X}) d\vec{X}}. \quad (13)$$

Where $\rho(\vec{X}, \vec{X})$ denotes the density matrix which can be got by replacing t with $-i\beta\hbar$ in Eq. (12).

Then applying Eq. (13), we obtain

$$\langle \vec{X}^2 \rangle = d \left[\frac{2m\omega}{\hbar} \tanh\left(\frac{\omega\beta\hbar}{2}\right) - \frac{2 \tanh^2\left(\frac{\omega\beta\hbar}{2}\right)}{\hbar^2 \omega^2 \left(\frac{\xi^2}{4\rho\eta^2 g} + \frac{\tanh \frac{\omega\beta\hbar}{2}}{\hbar m\omega^3} - \frac{\beta}{2m\omega^3} \right)} \right]^{-1}, \quad (14)$$

where

$$\omega = \left(\frac{2\rho\eta^2 g\beta}{m\xi^2} + \frac{\mu}{m} \right)^{1/2}. \quad (15)$$

RESULTS AND DISCUSSION

Figure 1, shows plot $\langle \tilde{X}^2 \rangle$ as a function of β , where the solid line corresponds to the replica method given in Eq. (1) and the dashed line corresponds to the path-integral method given in Eq. (14). It is shown in the graphs that the result of the path-integral method and the result of the replica method are in good agreement. Base on these results, we may conclude that the result of the path-integral method and the result of the replica method are exactly identical. However, in path-integral method, the mean square displacement is found to depend on the density of disorder, whereas this behavior does not occur in the replica method.

We now consider in case of the infinite-volume limit. As we discussed in the previous section that in order to mimic the effects of finite volume, the harmonic term was included in our model. Where μ is the strength of the harmonic potential and defines the system size (decreasing μ will increase the system size and when $\mu \rightarrow 0$ the system size goes to infinity). Thus, in case of the infinite volume limit, the particle does not see the confining harmonic potential. The behavior of a particle is determined only by the disorder. By taking the limit $\mu \rightarrow 0$ in Eq. (1) and in Eq. (14), we find that Eq. (1) diverges, whereas Eq. (14) is still finite. This indicates that the path-integral method still works in this case, but the replica method does not.

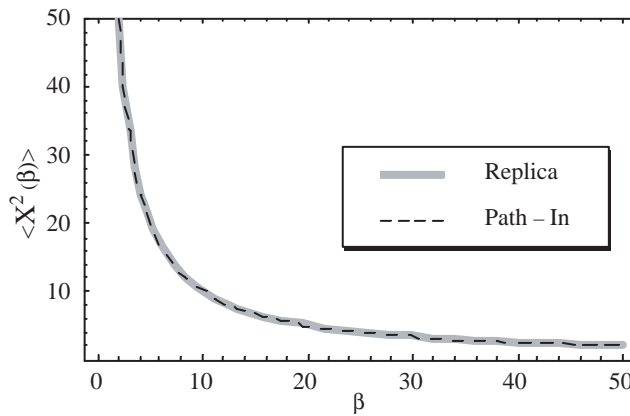


Figure 1 A plot of $\langle \tilde{X}^2 \rangle$ as a function of β . The parameters are $m = 9.1 \times 10^{-31}$, $\xi = 200$, $g = 0.1$, $d = 1$, $\mu = 0.01$, $\rho = 10^5$, $\hbar = 1.054 \times 10^{-34}$ and $\eta = 0.1$.

CONCLUSION

We have shown that the propagator and the mean square displacement of a quantum particle in random potential with long-range correlations can be exactly calculated using path-integral method without the replica.

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