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MEAN FIELD APPROACH TO THE RANDOM POTENTIAL PROBLEM

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Mean Field Approach to the Random Potential Problem

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ABSTRACT

The new method of the mean field type is proposed for the density of states calculation in the Gaussian random potential with Gaussian correlator. It becomes more precise when the dimension of space increases.

1. It has been known for a long time in the statistical physics of lattice systems the mean field approach leads to an adequate qualitative picture and gives good quantitative results up to the vicinity of a critical point [1]. Moreover, the availability and order of a phase transition can be predicted in the framework of this approach. Precision of the mean field description insreases with the particle number in a sphere of interaction. In the case of the nearest neighbours interaction this number increases with the space dimension D and in the limit $D\to\infty$ the mean field method becomes to be exact.

In this work the new approach to the density of states calculation in the Gaussian random potential with the Gaussian correlator is suggested. It becomes better when the space dimension increases. Concrete calculations are presented at $D=3$.

2. The Green function of Schrödinger equation averaged over the Gaussian random potential with the correlator:

$$\langle V(\vec{x})\,V(\vec{x}\,')\rangle = K(\vec{x}-\vec{x}\,') \qquad (1)$$

may be represented as a path integral [2]:

$$\langle G(\vec{x},T)\rangle = \int\limits_{\substack{\vec{x}(0)=0\\ \vec{x}(T)=\vec{x}}} D\vec{x}(t)\exp\left\{ i\int_0^T \frac{\dot{\vec{x}}^2}{2}\,dt - \frac{1}{2}\int_0^T\!\!\int_0^T dt\,dt'\,K(\vec{x}(t)-\vec{x}(t'))\right\}. \qquad (2)$$

For the density of states calculation it is enough to know $G(0;T)$:

$$\rho(\omega) = \langle \operatorname{Im} G(0, \omega) \rangle, \qquad G(0, \omega) = \int_{-\infty}^{+\infty} \frac{dT}{2\pi} e^{i\omega T} G(0, T) \tag{3}$$

i. e. to integrate in (2) over the closed paths. In what follows we will study the case when the correlator $K(\vec{x})$ is Gaussian:

$$K(\vec{x}) = K \exp(-\vec{x}^2/a^2). \tag{4}$$

The paths in multidimensional space restricted to a lower dimensional subspace have a zero measure in the integral (2). It is reasonable to suppose that the closed paths dominating in (2) are mainly isotropic. (More rigorous statements can be made in the simplest cases, see [3]). For such paths the average over trajectory $\langle \vec{x}(t)\vec{x}(t') \rangle$ has factor $1/D$:

$$\langle (\vec{x}\vec{x}')^2 \rangle = \frac{1}{D} \vec{x}^2 \vec{x}'^2 \tag{5}$$

and as a consequence the last multiplier in the product:

$$\exp\left[-\frac{(\vec{x}(t) - \vec{x}(t'))^2}{a^2}\right] = \exp\left(-\frac{\vec{x}^2(t) + \vec{x}^2(t')}{a^2}\right) \exp\left(\frac{2\vec{x}(t)\vec{x}(t')}{a^2}\right) \tag{6}$$

can be changed to 1 when $D \to \infty$. For example, we have when $D = 3$:

$$\frac{1}{\Omega\Omega'} \int \exp(\vec{x}\vec{x}')\, d\Omega\, d\Omega' = \frac{\operatorname{sh}(|\vec{x}|\,|\vec{x}'|)}{|\vec{x}|\,|\vec{x}'|}$$

and the right hand side at $|\vec{x}| = |\vec{x}'| = 1$ is equal to 1.18 just as $e^{-x^2} = 0.37$. In this case the first multiplier in (6) does determine behaviour of the full function. If in (2) the paths with $|\vec{x}| \gg a$ are dominate (in other words big fluctuations are essential) than our approximation fails. As a matter of fact, it's a general property of all the methods of mean field type.

When the last multiplier in (6) is changed to 1 the calculation of $\langle G(0, T) \rangle$ is been reduced to the averaging over one-parametric family of potentials:

$$\langle G(0, T) \rangle = \frac{1}{\sqrt{2\pi K}} \int d\alpha\, e^{-\alpha^2/2K} \int D\vec{x}(t) \exp\left[i \int_0^T dt \left(\frac{\dot{\vec{x}}^2}{2} + \frac{\alpha}{2} e^{-\vec{x}^2/a^2}\right)\right] =$$

$$= \frac{1}{\sqrt{2\pi K}} \int d\alpha\, e^{-\alpha^2/2K}\, \tilde{G}_\alpha(0, T) \tag{7}$$

where $\tilde{G}_\alpha(\vec{x}, T)$ is the Green function of the Schrödinger equation with the potential $\alpha \exp(-\vec{x}^2/a^2)$.

3. The completeness condition enables represent $\operatorname{Im} \tilde{G}_\alpha(0, T)$ as the series:

$$\rho_\alpha(\omega) = \sum_n |\psi_n(0)|^2 \delta(\omega - E_n) + \int_0^\infty dk\, |\psi_k(0)|^2 \delta\left(\omega - \frac{k^2}{2}\right) \tag{8}$$

where the summation over discrete and the integration over continue spectrum is implied. In what follows only the physical case $D = 3$ will be considered. The nonzero contribution in $\rho_\alpha(\omega)$ is given by the states with orbital momentum $l = 0$, i. e.

$$\psi_n(r) = \chi_n(r)/r$$

where E_n and $\chi_n(r)$ are eigenvalues and eigenfunctions of the radial Hamiltonian:

$$H_\alpha = -\frac{1}{2}\frac{d^2}{dr^2} + \alpha e^{-r^2/a^2} \tag{9}$$

and $\chi_n(0) = 0$. The Hamiltonian (9) does not belong to exactly diagonalizable. Nevetheless we can approximate it by another one with a rapidly decreasing potential, for example, by spherical well:

$$V_\alpha(r) = \begin{cases} \alpha, & r < a \\ 0, & r > a \end{cases} \tag{10}$$

The qualitative and rough quantitative structure of spectrum remains unchanged under this approximation. For the radial Hamiltonian H'_α:

$$H'_\alpha = -\frac{1}{2}\frac{d^2}{dr^2} + V_\alpha(r). \tag{11}$$

$\rho_\alpha(\omega)$ can be exactly calculated. The wave functions of continue spectrum ($\omega > 0$) in the region $r < a$ are equal to:

$$\alpha < \omega: \quad \psi_k = A \sin k_1 r / r,$$

$$k = \sqrt{2\omega}, \quad k_1 = \sqrt{2(\omega - \alpha)},$$

$$A^2=\frac{2}{\pi}\,\frac{k^2}{k_1^2+(k^2-k_1^2)\sin^2 k_1 a}; \tag{12}$$

$$\alpha>\omega: \quad \psi_k(r)=A\ \mathrm{sh}\ k_1 r/r,$$

$$k_1=\sqrt{2(\alpha-\omega)},$$

$$A^2=\frac{2}{\pi}\,\frac{k^2}{k_1^2+(k^2+k_1^2)\,\mathrm{sh}^2 k_1 a}. \tag{13}$$

The corresponding normalized wave functions in the region $r>a$ have a form:

$$\psi_k(r)=\sqrt{\frac{2}{\pi}}\,\sin(kr+\delta)/r \tag{14}$$

(see e. g. [4]). Thus when $\omega>0$ we have:

$$\langle\rho(\omega)\rangle=\frac{1}{2\pi^{5/2}}\sqrt{\frac{\omega}{K}}\left\{\int_{-\infty}^{\omega}d\alpha\, e^{-\alpha^2/2K}\,\frac{1}{1+\frac{\alpha}{\omega-\alpha}\sin^2(\sqrt{2(\omega-\alpha)}\,a)}+\right.$$

$$\left.+\int_{\omega}^{+\infty}d\alpha\, e^{-\alpha^2/2K}\,\frac{1}{1+\frac{\alpha}{\alpha-\omega}\,\mathrm{sh}^2(\sqrt{2(\alpha-\omega)}\,a)}\right\} \tag{15}$$

The asymptotic form of (15) when $\omega\to+\infty$:

$$\langle\rho(\omega)\rangle\approx\frac{1}{\pi^2}\sqrt{\frac{\omega}{2}} \tag{16}$$

gives the density of states for the free particle. When $\omega<0$ wave functions in the region $r<a$ are equal to:

$$\psi(r)=A\sin kr/r, \quad k=\sqrt{2(\omega-\alpha)} \quad \varkappa=\sqrt{2|\omega|},$$

$$A^2=\frac{2\varkappa}{\varkappa a+1} \tag{17}$$

where α is a zero of the function $k\cos ka+\varkappa\sin ka$. The averaged density of states at $\omega<0$ can be written as

$$\langle\rho(\omega)\rangle=\frac{1}{2\pi^{3/2}\sqrt{K}}\int_{-\infty}^{0}d\alpha\, e^{-\alpha^2/2K}\,\frac{\omega-\alpha}{|\sin\sqrt{2(\omega-\alpha)}\,a|}\times$$

$$\times\,\delta(\sqrt{\omega-\alpha}\cos(\sqrt{2(\omega-\alpha)}\,a)+\sqrt{|\omega|}\sin(\sqrt{2(\omega-\alpha)}\,a)). \tag{18}$$

When ω is arbitrary the compact form for $\langle\rho(\omega)\rangle$ exists:

$$\langle\rho(\omega)\rangle=\frac{1}{2\pi^{5/2}K^{1/2}}\,\mathrm{Re}\left\{\sqrt{\omega}\int_{-\infty}^{+\infty}d\alpha\, e^{-\alpha^2/2K}\,\frac{\omega-\alpha}{\omega-\alpha+\alpha\sin^2(\sqrt{2(\omega-\alpha)}\,a)+i0}\right\} \tag{19}$$

The sign of square root is defined by condition $\langle\rho(\omega)\rangle>0$. Note that the function $\langle\rho(\omega)\rangle$ is continuous at $\omega\to 0$ since the first integral in curly brackets in (15) behaves as $\omega^{-1/2}$ and we have

$$\langle\rho(0)\rangle=\frac{1}{8a^3}\sqrt{\frac{\pi}{2K}}\sum_{n=0}^{\infty}(2n+1)^2\exp\left[-\frac{\pi^4}{132Ka^4}(2n+1)^4\right]. \tag{20}$$

If Ka^4 is not large the first term does dominate:

$$\langle\rho(0)\rangle\approx\frac{1}{8a^3}\sqrt{\frac{\pi}{2K}}\exp\left(-\frac{\pi^4}{132Ka^4}\right). \tag{21}$$

If $Ka^4\gg 1$ the summation in (20) can be changed to the integration which results in:

$$\langle\rho(0)\rangle\approx\Gamma(3/4)\,2^{-5/4}\pi^{-5/2}K^{1/4}. \tag{22}$$

It coincides with the semiclassical expression (see e. g. [5]).

When $\omega<0$, $\omega^2\gg K$, $|\omega|\gg Ka^2$ the asymptotical expression for $\langle\rho(\omega)\rangle$ equals:

$$\langle\rho(\omega)\rangle=\frac{1}{2a^3}\sqrt{\frac{1}{2\pi K}}\exp\left[-\frac{1}{2K}\left(\omega^2+\frac{|\omega|\pi^2}{a^2}\right)\right]\times$$

$$\times\{1+O(e^{-3|\omega|\pi^2/a^2})\}. \tag{23}$$

If in the region $\omega<0$, $\omega^2\gg K$ the inequality $|\omega|\ll Ka^2$ takes place than the summation over all the zeros of the δ-function argument must be carried out. These zeros are:

$$\alpha_n\approx\omega-\frac{1}{2}\left(\frac{\pi n}{a}\right)^2 \tag{24}$$

and density of states

$$\langle\rho(\omega)\rangle\approx\frac{K}{4\pi^2|\omega|^{3/2}}\exp(-\omega^2/2K) \tag{25}$$

is also in agreement with the semiclassical result [5].

4. The approximation (10) is not sufficient for our approach and can be improved if necessary. E. g. the approximation proposed in [6] for the potential e^{-x^2/a^2} can be used, but the calculations become more sophisticated. The factorization in (6) when $D \to \infty$ takes place in the special case of Gaussian correlation function. For correlators with a power decreasing an other approach is required.

We can estimate the contribution from the first neglected term of the action in (2):

$$-\frac{K}{2a^2}\left(\int_0^T e^{-\vec{x}^2/a^2}\vec{x}\,dt\right)^2$$

It can be represented as the potential term:

$$-i\int_0^T \frac{\vec{\varphi}\vec{x}}{a}\,e^{-\vec{x}^2/a^2}\,dt \qquad (26)$$

averaged over vectors $\vec{\varphi}$ with the weight $\exp(-\vec{\varphi}^2/2K)$. The induced second-order shift of an energy level is equal to:

$$\delta E_n = \sum_{n'} \frac{1}{E_n - E_{n'}} \,|\langle n, l=0|\vec{x}e^{-\vec{x}^2/a^2}|n', l=1\rangle|^2.$$

For example, in the case $E_0 < 0$, $E_0^2 \gg K$, $|E_0| \gg Ka^2$ (corresponding $\langle\rho(\omega)\rangle$ is (23)) we have:

$$\delta E_0 \cdot a^2 \approx \pi^{-2} \cdot Ka^4.$$

The multiplier in front of the dimensionless parameter Ka^4 contains factor $1/D$, which comes from the fact that the sum rule:

$$\langle n|r^2|n\rangle = \sum_{n'} |\langle n|r|n'\rangle|^2$$

is not saturated by one fixed state $|n'\rangle$.

The density of states allows one to evaluate only the static characteristic as magnetic susceptibility, specific heat etc. For the kinetic ones the space dependence of Green function should be known; the present method requires some modification in this case.

The density of states asymptotics at $\omega \to -\infty$, $a \to \infty$ was calculated also in the work [7] with the help of the replica method and saturation of functional integral by instanton configurations. Off-exponential factor in [7] differs from that in (23) and from the semiclassical limit (25). It seems that this difference is the manifestation of imperfection of the replica trick and instanton approximation.

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