

Particle in a random potential: a new field-theory formulation

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A new representation of the Green's function of the Schrödinger equation is proposed. In this new representation, in the form of a functional integral, the problem of an electron in a random potential can be reduced to a field-theory problem without the use of a replica method or supersymmetry.

The problem of Anderson localization cannot be solved by perturbation theory.¹ Attempts have accordingly been made to formulate the problem of the motion of an electron in a random potential in terms of the field theory, which would make it possible to go beyond perturbation theory.^{2–4} In these studies, the electron Green's function has been represented as a functional integral over some field variable, and an average has initially been taken over random external potentials. This averaging gives rise to an effective nonlinear self-effect of the electron field, and the problem can be solved by field methods.

The Green's function of an electron in a random potential, $U(\mathbf{r})$ can be written in the energy representation as

$$G_E^{R,A}(\mathbf{r}_2, \mathbf{r}_1) = \pm i Z_{R,A}^{-1}(E) \int \mathcal{D}\psi \mathcal{D}\psi^* \psi(\mathbf{r}_2) \bar{\psi}(\mathbf{r}_1) \exp\{\pm i \int d\mathbf{r} \bar{\psi}(E - \hat{H} \pm i\delta)\psi\}, \quad (1)$$

$$Z_{R,A}(E) = \int \mathcal{D}\psi \mathcal{D}\bar{\psi} \psi^* \exp \{ \pm i \int dt \bar{\psi} (E - \hat{H} \pm i\delta) \psi \}, \quad (2)$$

where $\hat{H} = \hat{H}_0 + U(\mathbf{r})$, and \hat{H}_0 is the Hamiltonian of the free electron.

If the normalization denominator $Z_{R,A}$ were independent of U , it would be a trivial matter to average Green's function (1) (or the product of different Green's functions) in the Gaussian case. If, however, $\psi(\mathbf{r})$ is an ordinary one-component wave function, then we have

$$Z_{R,A}(E) \propto \exp \{ -\text{Tr} \ln(-i(E - \hat{H} \pm i\delta)) \} \propto \prod_{\lambda} (E - \epsilon_{\lambda} \pm i\delta)^{-1}, \quad (3)$$

where ϵ_{λ} are the eigenvalues of \hat{H} ; i.e., $Z_{R,A}$ depends on the potential. Wegner² has suggested eliminating this dependence by using a replica method, in which $\psi(\mathbf{r})$ is treated as an N -component vector, and the limit $N \rightarrow 0$ is taken in the final expression. Recent studies have shown, however, that the replica method used outside perturbation theory can lead to incorrect results.¹⁾

Another method for eliminating the denominator Z (a supersymmetry method) was proposed in Ref. 4. This method differs from the replica method in being mathematically rigorous. However, the introduction of Grassman variables in a problem without an interaction, in which the Fermi statistics of the electrons is not manifested, seems physically unjustified.

In the present letter we propose a new method for representing the field integral for the Green's function. In this new method, no additional field components are introduced; ψ has the clear physical meaning of a single-component wave function; and we have the denominator $Z_{R,A} \equiv 1$.

The introduction of a normalizing denominator in field theory corresponds to the cancellation of unconnected vacuum diagrams. It is clear, however, that in a one-particle problem (described by an ordinary Schrödinger equation) there can be no pair production, even virtual production. For this reason, if the functional integral is written correctly, there will be no need for a normalizing denominator. The same circumstance explains why the Feynman path integral⁵ also has no nontrivial normalizing denominator.

We write the Green's function in the time representation as a functional integral over time-dependent wave functions $\psi(\mathbf{r}, t)$:

$$G^{R,A}(x_2, x_1) = \pm Z_{R,A}^{-1} \int \mathcal{D}\psi \mathcal{D}\bar{\psi} \psi^*(x_2) \psi^*(x_1) \exp(\pm i \int dx \bar{\psi} \hat{L}^{R,A} \psi), \quad (4)$$

$$Z_{R,A} = \int \mathcal{D}\psi \mathcal{D}\bar{\psi} \psi^* \exp(\pm i \int dx \bar{\psi} \hat{L}^{R,A} \psi), \quad (5)$$

$$\hat{L}^{R,A} = i \partial_t - \hat{H} \pm i\delta; \quad x \equiv (\mathbf{r}, t). \quad (6)$$

If the functional integrals in (4) and (5) are to have a completely definite meaning,⁶ they must be understood as the limits of finite-dimensional integrals, which arise upon the introduction of the discrete time $t_n = n\Delta$, where $n = -N, \dots, N$. The integration over the time t is replaced by a summation over n , and the operators $\hat{L}^{R,A}$ are the limits of the finite-dimensional matrices

$$\tilde{L}_{nn'}^{R,A} = \pm i(\delta_{n'n} - \delta_{n'n \mp 1}) - \Delta(\hat{H}_{n \mp 1/2} \mp i\delta)\delta_{n'n \mp 1}. \quad (7)$$

These matrices are triangular; $\tilde{L}^{R+} = \tilde{L}^A$; and in \tilde{L}^R all the elements above the diagonal are zero, while in \tilde{L}^A all the elements below the diagonal are zero. It is thus clear (this point can be proved rigorously) that L^R generates a retarded Green's function, while L^A generates a leading Green's function:

$$\tilde{G}^{R,A} = (\tilde{L}^{R,A})^{-1}; \quad G^{R,A} = \lim_{\Delta \rightarrow 0, N \rightarrow \infty} \tilde{G}^{R,A}. \quad (8)$$

The determinant of a triangular matrix is equal to the product of its diagonal elements, so we have $\det(\tilde{L}^{R,A}) = (\pm i)^{2N+1} \neq 0$. This condition ensures the existence and uniqueness of the inverse matrices in (8), which we need if representation (4) is to be meaningful. If we define the measure in integrals (4) and (5) as

$$\mathcal{D}\psi \mathcal{D}\psi^* \equiv \prod_{n=-N}^N \pi^{-1} D \operatorname{Re} \psi(\mathbf{r}, t_n) D \operatorname{Im} \psi(\mathbf{r}, t_n), \quad (9)$$

then we have

$$\tilde{Z}_{R,A} = \det(\mp i L^{R,A}) = 1, \quad Z_{R,A} = \lim_{\Delta \rightarrow 0, N \rightarrow \infty} \tilde{Z}_{R,A} = 1. \quad (10)$$

We have thus shown that expression (4) can be written without any normalization denominator at all. This circumstance means that taking a Gaussian average over U is a trivial matter in representation (4).

All these arguments apply to a Hamiltonian $\hat{H}(t)$, which depends on the time in an arbitrary way. In the case of a static Hamiltonian \hat{H} , we write (4) and (5) in the energy representation and find

$$G_E^{R,A}(\mathbf{r}_2, \mathbf{r}_1) = \mp i \int D\psi D\psi^* \psi_E(\mathbf{r}_2) \psi_E^*(\mathbf{r}_1) \exp\{\pm i \int dE' d\mathbf{r} \psi_{E'}^*(E' - \hat{H} \pm i\delta) \psi_{E'}\}. \quad (11)$$

In the energy representation, condition (10) becomes

$$1 = Z_{R,A} \propto \prod_{E'} Z_{R,A}(E') = \prod_{\lambda} \prod_{E'} (E' - \epsilon_{\lambda} \pm i\delta)^{-1}. \quad (12)$$

Since all the singularities of (12) lie in the same half-plane of the complex variable E' , we see that the latter product is actually independent of ϵ_{λ} . To prove this assertion rigorously, we must transform (10) to the energy representation for finite Δ and N and take the limit only after the subtraction of the product. From (12) we have $Z_{R,A}^{-1}(E) \propto \prod_{E' \neq E} Z_{R,A}(E')$; using (2), we can then easily prove that definitions (1) and (11) are identical.

Consequently, in order to avoid a nontrivial normalization factor, we must replace the functional integration over $\psi(\mathbf{r})$, which depends on only \mathbf{r} , by an integration over $\psi(\mathbf{r}, t)$ or over $\psi_{E'}(\mathbf{r})$, i.e., over wave functions corresponding to all energies.

The generating functional, which generates arbitrary products of G^R and G^A , averaged over a Gaussian admixture potential, is

$$Z(\rho_R, \rho_A) = \int (\hat{\mathcal{D}}) U(\hat{\mathcal{L}}\psi) \exp \left\{ i \int dx (\psi_R^* \hat{L}^R \psi_R - \psi_A^* \hat{L}^A \psi_A + \rho_R^* \psi_R + \psi_R^* \rho_R - \rho_A^* \psi_A - \psi_A^* \rho_A) - \frac{1}{2} \int d\mathbf{r} d\mathbf{r}' U(\mathbf{r}) \gamma^{-1}(\mathbf{r} - \mathbf{r}') U(\mathbf{r}') \right\}, \quad (13)$$

where $\gamma(\mathbf{r} - \mathbf{r}')$ is the correlation function of the random potentials, and the integration is carried out independently over $\psi_R(x)$ and $\psi_A(x)$; here $(D\psi) \equiv D\psi_R D\psi_R^* D\psi_A D\psi_A^*$. After integrating over U and using (5) and (10), we find

$$Z(\rho_R, \rho_A) = \int (\hat{\mathcal{D}}\psi) \exp \left\{ i S_{eff} + i \int dx [(\bar{\rho}\psi) + (\bar{\psi}\rho)] \right\}, \quad (14)$$

$$S_{eff} = \int dx (\bar{\psi} \hat{L}_0 \psi) + \frac{i}{2} \iint dx dx' (\bar{\psi}\psi)_x \gamma(\mathbf{r} - \mathbf{r}') (\bar{\psi}\psi)_{x'}, \quad (15)$$

$$\psi = \begin{pmatrix} \psi_R \\ \psi_A \end{pmatrix}, \quad \rho = \begin{pmatrix} \rho_R \\ \rho_A \end{pmatrix}, \quad \bar{\psi} = (\psi_R^*, -\psi_A^*), \quad \bar{\rho} = (\rho_R^*, -\rho_A^*), \quad (16)$$

$$\hat{L}_0 = \begin{pmatrix} \hat{L}_0^R & 0 \\ 0 & \hat{L}_0^A \end{pmatrix}, \quad (17)$$

where $\hat{L}_0^{R,A}$ corresponds to $U = 0$. The two-particle Green's function associated with the density-density correlation function can be expressed in terms of the generating functional as follows:

$$\langle G^R(x_2 x_1) G^A(x'_2 x'_1) \rangle = \frac{\delta^4 Z(\rho_R, \rho_A)}{\delta \rho_A(x'_1) \delta \rho_A^*(x'_2) \delta \rho_R^*(x_2) \delta \rho_R(x_1)} \Big|_{\rho=0}. \quad (18)$$

Expressions for more complex correlation functions can be written in an analogous way.

Expression (15), derived for a random static potential, is in direct correspondence with the expression derived in Ref. 7 for a time-dependent random potential (phonons). The presence of a correlation between wave functions at all times (for all energies) in (15) is a consequence of the static nature of the potential, and it reflects the fact that the expression for the Green's function of the Schrödinger equation at a given energy contains eigenfunctions corresponding to all energies.

As in Refs. 2 and 3, we could introduce collective variables (Q -matrices) in integral (14) by means of the Hubbard-Stratonovich transformation, but in our case the Q -matrices can describe the correlation between wave functions for different energies: $Q_{EE'} \propto \langle \psi_E \bar{\psi}_{E'} \rangle$.

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