Path integral scheme on a flexible time contour for random electron models

1988 J. Phys. A: Math. Gen. 21 L333

(http://iopscience.iop.org/0305-4470/21/6/003)

J. Phys. A: Math. Gen. 21 (1988) L333-L337. Printed in the UK

LETTER TO THE EDITOR

Path integral scheme on a flexible time contour for random electron models

E Kolley and W Kolley

Sektion Physik, Karl Marx Universität, DDR-7010 Leipzig, German Democratic Republic

Received 2 December 1987

Abstract. A field-theoretic time path approach to an interacting electron system with quenched site randomness is extended to a one-parameter variety of contours. The average generating functional for real-time finite-temperature Green functions is deduced. Propagators along the Keldysh contour and the Niemi–Semenoff contour are included as special cases.

Time path ordered formulations [1-8] of the real-time finite-temperature field theory can be established by functional-integral representations [3-8] (especially for fermions [4, 6-8] and with quenched disorder [7, 8]) along the Keldysh contour [1, 2, 7, 8] or the Niemi–Semenoff contour [3, 4, 6]. Another approach achieved by operator doubling concerns thermofield dynamics [9, 10]. Within the time path framework a contour varying by a free parameter as in [5, 9, 11] is allowed due to analyticity. In this letter we extend the tight-binding version [8] to such a more general contour.

Consider an electron system in the presence of disorder and interaction. The generating functional for real-time thermal Green functions can be represented by the path integral (cf [8])

$$Z[\bar{\chi}, \chi] = \frac{1}{Z} \int \mathscr{D}\bar{c}\mathscr{D}c \, \exp[\mathrm{i}(A[\bar{c}, c] + \bar{c}\chi + \bar{\chi}c)] \tag{1}$$

over Grassmann variables $\bar{c}_{i\sigma}(t)$ and $c_{i\sigma}(t)$ at lattice site i, spin σ and time t, so that

$$\mathscr{D}\bar{c}\mathscr{D}c = \prod_{i\sigma, t \in \mathscr{C}_{\sqsupset}} \mathscr{D}\bar{c}_{i\sigma}(t)\mathscr{D}c_{i\sigma}(t).$$

The time contour $\mathscr{C}_{\sqsupset}$ chosen here (see figure 1) consists of four segments: $\mathscr{C}^{(1)}(t_a \to t_b)$ along the real axis, $\mathscr{C}^{(3)}(t_b \to t_b - \mathrm{i}\nu)$ parallel to the imaginary axis, $\mathscr{C}^{(2)}(t_b - \mathrm{i}\nu \to t_b - \mathrm{i}\nu)$ parallel to the real axis, and $\mathscr{C}^{(4)}(t_a - \mathrm{i}\nu \to t_a - \mathrm{i}\beta)$ parallel to the imaginary axis, where $\nu \in (0, \beta)$ with β being the inverse temperature. The partition function Z is defined by the normalisation $Z[0,0] = 1$. The action in (1) is given by

$$A[\bar{c}, c] = \int_{\mathscr{C}_{\sqsupset}} \mathrm{d}t \left(\sum_{i\sigma} \bar{c}_{i\sigma} \mathrm{i} \frac{\partial}{\partial t} c_{i\sigma} - \mathscr{H}[\bar{c}(t), c(t)] \right) \tag{2}$$

in terms of the Hamiltonian $\mathscr{H}$ including the chemical potential. The anticommuting sources $\bar{\chi}$ and χ are assumed to be absent on $\mathscr{C}^{(3)}$ and $\mathscr{C}^{(4)}$, i.e.

$$\bar{c}\chi = \int_{\mathscr{C}^{(1)} + \mathscr{C}^{(2)}} \mathrm{d}t \sum_{i\sigma} \bar{c}_{i\sigma}(t)\chi_{i\sigma}(t).$$

0305-4470/88/060333+05$02.50

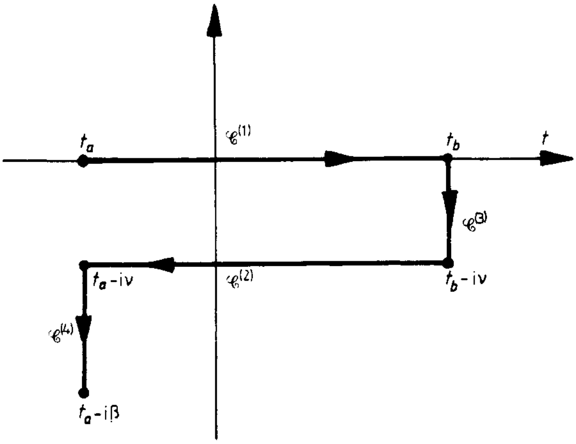

Figure 1. The time contour $\mathscr{C}_{\sqsupset}$.

The fermionic boundary conditions to (1) are

$$c_{i\sigma}(t_a)=-c_{i\sigma}(t_a-i\beta) \qquad \bar{c}_{i\sigma}(t_a)=-\bar{c}_{i\sigma}(t_a-i\beta). \tag{3}$$

We treat first the non-random and non-interacting case. Then, instead of (2), the unperturbed action A_0 enters the exponent of (1) after the spatial Fourier transformation as

$$A_0[\bar{c},c]+\bar{c}\chi+\bar{\chi}c$$
$$=\int_{\mathscr{C}_{\sqsupset}} dt \sum_{k\sigma} \bar{c}_{k\sigma}\left(i\frac{\partial}{\partial t}-\tilde{\varepsilon}_k\right)c_{k\sigma}+\int_{\mathscr{C}^{(1)}+\mathscr{C}^{(2)}} dt \sum_{k\sigma} (\bar{c}_{k\sigma}\chi_{k\sigma}+\bar{\chi}_{k\sigma}c_{k\sigma}) \tag{4}$$

where $\tilde{\varepsilon}_k=\varepsilon_k-\mu$ involves the band energy

$$\varepsilon_k=\frac{1}{N}\sum_{\substack{ij\\(i\neq j)}} t_{ij}\exp[-ik(\boldsymbol{R}_i-\boldsymbol{R}_j)]$$

where t_{ij} is the periodic hopping integral, μ the chemical potential and N the number of sites. On the basis of (4) the resulting Gaussian functional integral for $Z_0[\bar{\chi},\chi]$ is determined by the extremal trajectory which satisfies the equations of motion

$$i\frac{\partial}{\partial t}c_{k\sigma}^{(\alpha)}-\tilde{\varepsilon}_k c_{k\sigma}^{(\alpha)}=\begin{cases}-\chi_{k\sigma}^{(\alpha)} & \alpha=1,2\\ 0 & \alpha=3,4\end{cases} \tag{5}$$

where α refers to time arguments on the segment $\mathscr{C}^{(\alpha)}$. Analogous equations hold for $\bar{c}_{k\sigma}^{(\alpha)}$ but with $\partial/\partial t$ replaced by $-\partial/\partial t$. In solving (5) the fields on $\mathscr{C}^{(3)}$ and $\mathscr{C}^{(4)}$ can be eliminated via matching conditions at the points t_b, $t_b-i\nu$ and $t_a-i\nu$. In particular, (3) becomes

$$c_{k\sigma}^{(1)}(t_a)=-\exp[-(\beta-\nu)\tilde{\varepsilon}_k]c_{k\sigma}^{(2)}(t_a-i\nu) \qquad \bar{c}_{k\sigma}^{(1)}(t_a)=-\exp[(\beta-\nu)\tilde{\varepsilon}_k]\bar{c}_{k\sigma}^{(2)}(t_a-i\nu). \tag{6}$$

The solution of (5) at $\alpha=1$, 2, under the first boundary condition of (6) and under the constraint

$$c_{k\sigma}^{(1)}(t_b)=\exp\{\nu\tilde{\varepsilon}_k\}c_{k\sigma}^{(2)}(t_b-i\nu)$$

is given by

$$\begin{pmatrix} c^{(1)}_{k\sigma}(t) \\ c^{(2)}_{k\sigma}(t-\mathrm{i}\nu) \end{pmatrix} = -\mathrm{i}\int_{t_a}^{t_b} \mathrm{d}t' \exp[-\mathrm{i}\tilde{\varepsilon}_k(t-t')] \times \begin{pmatrix} -\vartheta(t-t')+f(\tilde{\varepsilon}_k) & -\exp(\nu\tilde{\varepsilon}_k)f(\tilde{\varepsilon}_k) \\ -\exp(-\nu\tilde{\varepsilon}_k)(1-f(\tilde{\varepsilon}_k)) & \vartheta(t'-t)-f(\tilde{\varepsilon}_k) \end{pmatrix} \begin{pmatrix} \chi^{(1)}_{k\sigma}(t') \\ \chi^{(2)}_{k\sigma}(t'-\mathrm{i}\nu) \end{pmatrix} \tag{7a}$$

with the step function $\vartheta(t-t')$ and the Fermi distribution $f(\tilde{\varepsilon}_k)=[\exp(\beta\tilde{\varepsilon}_k)+1]^{-1}$. Let us abbreviate (7*a*) by

$$c = -\hat{\mathbf{G}}_0\sigma_3\chi \tag{7b}$$

with

$$\sigma_3 = \begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix}.$$

The 2×2 matrix $\hat{\mathbf{G}}_0$ from (7*a*) takes for $t_a\to-\infty$ and $t_b\to\infty$ the Fourier transform

$$\hat{\mathbf{G}}_{0,k}(\omega) = \begin{pmatrix} (1-f(\tilde{\varepsilon}_k))\mathbf{G}^r_{0,k}(\omega)+f(\tilde{\varepsilon}_k)\mathbf{G}^a_{0,k}(\omega) & -\exp(\nu\tilde{\varepsilon}_k)f(\tilde{\varepsilon}_k)(\mathbf{G}^r_{0,k}(\omega)-\mathbf{G}^a_{0,k}(\omega)) \\ \exp(-\nu\tilde{\varepsilon}_k)(1-f(\tilde{\varepsilon}_k))(\mathbf{G}^r_{0,k}(\omega)-\mathbf{G}^a_{0,k}(\omega)) & -f(\tilde{\varepsilon}_k)\mathbf{G}^r_{0,k}(\omega)-(1-f(\tilde{\varepsilon}_k))\mathbf{G}^a_{0,k}(\omega) \end{pmatrix} \tag{8}$$

where

$$\mathbf{G}^{a\,r}_{0,k}(\omega) = (\omega-\tilde{\varepsilon}_k\pm\mathrm{i}0)^{-1}$$

correspond to retarded (r) and advanced (a) Greenians. The ν dependence of the unperturbed propagator (8) leads for $\nu=0$ to the Keldysh matrix [1] structure

$$\hat{\mathbf{G}}_{0,k}(\omega)|_{\nu=0} = \begin{pmatrix} 1 & f(\omega) \\ 1 & -(1-f(\omega)) \end{pmatrix}\begin{pmatrix} \mathbf{G}^r_{0,k}(\omega) & 0 \\ 0 & \mathbf{G}^a_{0,k}(\omega) \end{pmatrix}\begin{pmatrix} 1-f(\omega) & -f(\omega) \\ 1 & 1 \end{pmatrix} \equiv \hat{a}(\omega)\hat{\mathbf{G}}^{\mathrm{dia}}_{0,k}(\omega)\hat{b}(\omega) \tag{9}$$

and in the symmetric case $\nu=\beta/2$ to

$$\hat{\mathbf{G}}_{0,k}|_{\nu=\beta/2} = \hat{w}(\omega)\hat{\mathbf{G}}^{\mathrm{dia}}_{0,k}(\omega)\sigma_3\hat{w}(\omega)$$

with

$$\hat{w}(\omega) = \begin{pmatrix} (1-f(\omega))^{1/2} & -(f(\omega))^{1/2} \\ (f(\omega))^{1/2} & (1-f(\omega))^{1/2} \end{pmatrix}. \tag{10}$$

Combining (1), (4), (5) and (7*b*) one gets the free generating functional

$$Z_0[\bar{\chi},\chi] = \exp\left(-\mathrm{i}\int_{-\infty}^{\infty}\mathrm{d}t\,\mathrm{d}t'\sum_{k\sigma}\bar{\chi}_{k\sigma}(t)\sigma_3\hat{\mathbf{G}}_{0,k}(t-t')\sigma_3\chi_{k\sigma}(t)\right) \equiv \exp(-\mathrm{i}\bar{\chi}\sigma_3\hat{\mathbf{G}}_0\sigma_3\chi) \tag{11}$$

with the doublet $\bar{\chi}(t)=(\bar{\chi}^{(1)}(t),\,\bar{\chi}^{(2)}(t-\mathrm{i}\nu))$.

We now incorporate both site disorder and on-site interaction as in [8]. In the limit $t_a\to-\infty$ and $t_b\to\infty$ the functional (1) can be factorised (cf [3-6, 8]) as

$$Z[\bar{\chi},\chi] = (1/Z)Z[\bar{\chi},\chi;\mathscr{C}^{(1)},\mathscr{C}^{(2)}]Z[0,0;\mathscr{C}^{(3)},\mathscr{C}^{(4)}] = Z[\bar{\chi},\chi;\mathscr{C}^{(1)},\mathscr{C}^{(2)}]. \tag{12}$$

This implies the normalisation $Z[0,0;\mathscr{C}^{(1)},\mathscr{C}^{(2)}]=1$. The remaining $Z[\bar{\chi},\chi;\mathscr{C}^{(1)},\mathscr{C}^{(2)}]$ stemming only from the horizontal segments can be expressed by

$$Z[\bar{\chi},\chi]=\int \mathscr{D}\bar{c}\mathscr{D}c\,\exp[\mathrm{i}(\bar{c}\hat{\mathbf{G}}_0^{-1}c+A_{\mathrm{ran}}[\bar{c},c]+A_{\mathrm{int}}[\bar{c},c]+\bar{c}\sigma_3\chi+\bar{\chi}\sigma_3 c)] \tag{13}$$

in doublet notation with

$$\mathscr{D}\bar{c}\mathscr{D}c=\prod_{\mathrm{i}\sigma,t\in(-\infty,\infty)}\mathscr{D}\bar{c}^{(1)}_{\mathrm{i}\sigma}(t)\mathscr{D}c^{(1)}_{\mathrm{i}\sigma}(t)\mathscr{D}\bar{c}^{(2)}_{\mathrm{i}\sigma}(t-\mathrm{i}\nu)\mathscr{D}c^{(2)}_{\mathrm{i}\sigma}(t-\mathrm{i}\nu).$$

Here we specify

$$A_{\mathrm{ran}}[\bar{c},c]=-\int_{-\infty}^{\infty}\mathrm{d}t\sum_{\mathrm{i}\sigma}\varepsilon_{\mathrm{i}}\bar{c}_{\mathrm{i}\sigma}(t)\sigma_3 c_{\mathrm{i}\sigma}(t) \tag{14}$$

$$A_{\mathrm{int}}[\bar{c},c]=-U\int_{-\infty}^{\infty}\mathrm{d}t\sum_{\mathrm{i}}[n^{(1)}_{\mathrm{i}\uparrow}(t)n^{(1)}_{\mathrm{i}\downarrow}(t)-n^{(2)}_{\mathrm{i}\uparrow}(t-\mathrm{i}\nu)n^{(2)}_{\mathrm{i}\downarrow}(t-\mathrm{i}\nu)] \tag{15}$$

to the Gaussian distribution

$$P(\varepsilon_{\mathrm{i}})=(1/2\pi\gamma)\exp(-\varepsilon_{\mathrm{i}}^2/2\gamma)$$

and to Hubbard's interaction in terms of $n^{(\alpha)}_{\mathrm{i}\sigma}=\bar{c}^{(\alpha)}_{\mathrm{i}\sigma}c^{(\alpha)}_{\mathrm{i}\sigma}$. There is no denominator problem. Weighting (13) by $\int\Pi_{\mathrm{i}}[\mathrm{d}\varepsilon_{\mathrm{i}}\,P(\varepsilon_{\mathrm{i}})]\ldots$ one finds the quenched-averaged generating functional

$$\bar{\bar{Z}}[\bar{\chi},\chi]=Z[\bar{\chi},\chi]|_{A_{\mathrm{ran}}\to\tilde{A}}$$

where

$$\tilde{A}[\bar{c},c]=\frac{\mathrm{i}\gamma}{2}\sum_{\mathrm{i}}\left(\int_{-\infty}^{\infty}\mathrm{d}t\sum_{\sigma}\bar{c}_{\mathrm{i}\sigma}(t)\sigma_3 c_{\mathrm{i}\sigma}(t)\right)^2. \tag{16}$$

To conclude, the path integral approach [8] to the dynamics of electrons within a random Hubbard model at finite temperature was extended to a variable (by the parameter ν) time contour. Compare the free thermal propagator matrices: (i) at arbitrary ν, (8) is the exact Fermi counterpart to the corresponding Bose result in [9]; (ii) at $\nu=0$, (9) is in agreement with [7, 8]; (iii) at $\nu=\beta/2$, the form (10) resembles the free propagator of Dirac fermions in [4]. As shown in [9] the case $\nu=\beta/2$ corresponds to thermofield dynamics. In the zero-temperature limit, $\hat{\mathbf{G}}_0$ becomes triangular (diagonal) for $\nu=0$ ($\beta/2$). Gaussian bond randomness around the non-zero average hopping may be included in the present formalism, where $\tilde{A}$ in (16) becomes non-local via a new variance γ_{ij} instead of γ. We have formulated a general as well as a flexible frame to construct a real-time field theory for disordered thermal fermions. The one-parameter family of time paths covers both the Keldysh and the Niemi-Semenoff contours. This is a step towards a unified dynamic description. At first glance such a time path concept seems to be formal or artificial. The advantage of the dynamic approach to disordered interacting electron systems consists of the possibility of avoiding the denominator problem. Thus, the quenched average can be carried out directly on the generating functional without replica trick or supersymmetry method; the latter would be restricted to the non-interacting case. The price one pays is the doubling of the degrees of freedom, but this emerges naturally from the positive and negative time directions. Moreover, thermal effects are taken into account straightforwardly. The interplay between disorder and interaction is of particular interest for electron localisation, itinerant spin glasses and their mutual influence. Our resulting effective action may serve as a basis to establish, without resource to the replica method, order parameters in the form of dynamic Q-matrix fields.

An interesting discussion with Professor L V Keldysh is gratefully acknowledged.

References

[1] Keldysh L V 1964 *Zh. Eksp. Teor. Fiz.* **47** 1515 (Engl. transl. 1965 *Sov. Phys.-JETP* **20** 1018)
[2] Rammer J and Smith H 1986 *Rev. Mod. Phys.* **58** 323
[3] Neimi A J and Semenoff G W 1984 *Ann. Phys., NY* **152** 105
[4] Kobes R L, Semenoff G W and Weiss N 1985 *Z. Phys.* C **29** 371
[5] Sakagami M and Kubota T 1986 *Prog. Theor. Phys.* **76** 548
[6] Kowalski K L 1987 *Phys. Rev.* D **35** 2415
[7] Babichenko V S and Kozlov A N 1986 *Solid State Commun.* **59** 39
[8] Kolley E and Kolley W 1987 *Phys. Lett.* **124A** 330
[9] Matsumoto H, Nakano Y, Umezawa H, Mancini F and Marinaro M 1983 *Prog. Theor. Phys.* **70** 599
[10] Matsumoto H, Mancini F and Marinaro M 1987 *Europhys. Lett.* **4** 153
[11] Lim S C 1987 *Phys. Lett.* **188B** 239