Continuous-Time Quantum Monte Carlo Algorithm for the Lattice Polaron

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An efficient continuous-time path-integral quantum Monte Carlo algorithm for the lattice polaron is presented. It is based on Feynman's integration of phonons and subsequent simulation of the resulting single-particle self-interacting system. The method is free from the finite-size and finite-time-step errors and works in any dimensionality and for any range of electron-phonon interaction. The ground-state energy and effective mass of the polaron are calculated for several models. The polaron spectrum can be measured directly by Monte Carlo, which is of general interest. [S0031-9007(98)07859-4]

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The past few years have witnessed a rapid development of continuous-time quantum Monte Carlo (QMC) algorithms for quantum-mechanical lattice models. The driving force behind this is the desire to eliminate the systematic errors introduced by the Trotter decomposition in the standard discrete-time QMC methods [1]. The main idea then is to regard the imaginary-time evolution of a particle or spin configuration as a continuous-time Poisson process with "events" being either a particle jump or a spin flip. In this way continuous-time QMC algorithms were developed for a particle in an external potential [2], Heisenberg model [3,4], *t-J* model [5], bosonic Hubbard model [6], and Fröhlich polaron [7].

In this Letter I present a continuous-time path-integral QMC algorithm for the lattice polaron, i.e., an electron strongly interacting with phonons on a lattice. The method combines analytical integration of the phonon degrees of freedom with the advantages of the continuous-time formulation of the Monte Carlo process. The method is universal. It works for infinite lattices in any dimensionality and for any radius of electron-phonon interaction. It is also free from the systematic finite-time-step errors which were an undesirable feature of the original (discrete-time) QMC algorithm based on the integration of phonons [8]. In fact, the new method allows for *exact* (in the QMC sense) calculation of the ground-state energy, effective mass, and even *spectrum* of the polaron. The numerical accuracy of the method is 0.1%–0.3%, which is not as good as that of exact diagonalization [9,10] and density-matrix renormalization group [11] schemes, but is good enough for practical purposes.

I begin with the important question of which quantities can be calculated with a path-integral QMC method. The traditional scheme samples paths which are periodic in imaginary time, see, e.g., Refs. [1,8]. This allows for the calculation of thermodynamic properties such as internal energy or specific heat, as well as some static correlation functions, but not dynamic properties of the system. In Ref. [12] it was shown that the polaron effective mass, an important dynamic characteristic, can be measured on the ensemble of paths with *open* boundary conditions in imaginary time (BCIT). Here I extend the argument to the whole polaron spectrum. Consider two quantities. The first one, $Z_{\mathbf{P}} = \sum_i \langle i|e^{-\beta H}|i\rangle \delta_{\mathbf{P}_i,\mathbf{P}}$, is by definition the partition function of many-body states with fixed total (electron plus phonon) quasimomentum $\mathbf{P}$ [$\beta = (k_B T)^{-1}$ and H is the Hamiltonian]. The second quantity is the partition function with twisted BCIT, $Z_{\Delta\mathbf{r}} = \mathrm{Tr}_{\Delta\mathbf{r}} e^{-\beta H}$, in which the many-body configurations (electron position $\mathbf{r}$ and ionic displacements $\vec{\xi}$) at $\tau = \beta$ are obtained from the configurations at $\tau = 0$ by shifting along the lattice by the vector $\Delta\mathbf{r}$. There exists a fundamental Fourier-type relation between the two [12]:

$$Z_{\mathbf{P}} = \sum_{\Delta\mathbf{r}} e^{i\mathbf{P}\Delta\mathbf{r}} Z_{\Delta\mathbf{r}} = \int_{\mathrm{op}} \mathcal{D}\mathbf{r}\, \mathcal{D}\vec{\xi}\, e^{i\mathbf{P}\Delta\mathbf{r}} w[\mathbf{r}(\tau)\vec{\xi}(\tau)]\,. \tag{1}$$

Here $w[\mathbf{r}(\tau)\vec{\xi}(\tau)]$ is the (positive-definite) weight of a many-body path satisfying the twisted BCIT, and $\int_{\mathrm{op}} \mathcal{D}\mathbf{r}\, \mathcal{D}\vec{\xi}$ means the integration over such paths with all possible shifts $\Delta\mathbf{r}$. In the low-temperature limit, $\beta \to \infty$, $Z_{\mathbf{P}}$ is dominated by the lowest eigenstate $E_{\mathbf{P}}$: $Z_{\mathbf{P}} = \exp(-\beta E_{\mathbf{P}})$ and $E_{\mathbf{P}} = -\frac{1}{Z_{\mathbf{P}}} \frac{\partial Z_{\mathbf{P}}}{\partial \beta}$. Equation (1) then gives

$$E_{\mathbf{P}} = \frac{\int_{\mathrm{op}} \mathcal{D}\mathbf{r}\, \mathcal{D}\vec{\xi}\, e^{i\mathbf{P}\Delta\mathbf{r}} [-\frac{1}{w}\frac{\partial w}{\partial \beta}] w}{\int_{\mathrm{op}} \mathcal{D}\mathbf{r}\, \mathcal{D}\vec{\xi}\, e^{i\mathbf{P}\Delta\mathbf{r}} w} \equiv \frac{\langle -e^{i\mathbf{P}\Delta\mathbf{r}} \frac{1}{w}\frac{\partial w}{\partial \beta}\rangle_0}{\langle e^{i\mathbf{P}\Delta\mathbf{r}}\rangle_0}\,, \tag{2}$$

where $\langle A\rangle_0 \equiv (\int_{\mathrm{op}} \mathcal{D}\mathbf{r}\, \mathcal{D}\vec{\xi}\, w)^{-1} \int_{\mathrm{op}} \mathcal{D}\mathbf{r}\, \mathcal{D}\vec{\xi}\, Aw$ stands for the average in the case $\mathbf{P} = 0$. Equation (2) shows that the ground-state dispersion of the polaron can be inferred *directly* from imaginary-time simulations. However, the formalism is not free from the sign problem, as apparent from Eq. (2). Energies for nonzero values of $\mathbf{P}$ can be obtained only at intermediate and large electron-phonon couplings when the average $\langle e^{i\mathbf{P}\Delta\mathbf{r}}\rangle_0 = \langle \cos \mathbf{P}\Delta\mathbf{r}\rangle_0$ is not small. The ground state corresponds to $\mathbf{P} = 0$ and its energy can be calculated straightforwardly using Eq. (2).

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Analogous formulas can be obtained for derivatives of $E_{\mathbf{P}}$ with respect to momentum, e.g., for the inverse effective mass. In the low-temperature limit one can write $E_{\mathbf{P}} = -\frac{1}{\beta}\ln Z_{\mathbf{P}}$ since there is no difference between $1/\beta$ and $\partial/\partial\beta$. From this and Eq. (1), it follows that

$$\frac{1}{m^*_\alpha} \equiv \frac{1}{\hbar^2}\frac{\partial^2 E_{\mathbf{P}}}{\partial P_\alpha^2}\bigg|_{\mathbf{P}=0} = \frac{\int_{\mathrm{op}} \mathcal{D}\mathbf{r}\,\mathcal{D}\vec{\xi}\,[\frac{(\Delta r_\alpha)^2}{\hbar^2\beta}]w}{\int_{\mathrm{op}} \mathcal{D}\mathbf{r}\,\mathcal{D}\vec{\xi}\,w} = \frac{\langle(\Delta r_\alpha)^2\rangle_0}{\hbar^2\beta}. \tag{3}$$

One can see that the inverse effective mass is the "diffusion coefficient" of the imaginary-time propagation. (For similar treatment of the continuous polaron and of an atom of ^{3}He in liquid ^{4}He, see [13] and [14], respectively.)

Thus, to compute dynamical properties, the QMC process should sample paths with open BCIT. Consider now a particular polaron system on a hypercubic lattice with nearest-neighbor hopping. The model is defined by the Hamiltonian

$$H = -t\sum_{\mathbf{n}\mathbf{n}'} c^\dagger_{\mathbf{n}'}c_{\mathbf{n}} - \sum_{\mathbf{m}\mathbf{n}} f_{\mathbf{m}}(\mathbf{n})c^\dagger_{\mathbf{n}}c_{\mathbf{n}}\xi_{\mathbf{m}} + \hbar\omega\sum_{\mathbf{m}} b^\dagger_{\mathbf{m}}b_{\mathbf{m}}. \tag{4}$$

The phonon subsystem (operators $b^\dagger_{\mathbf{m}}, b_{\mathbf{m}}$) is a set of uncoupled harmonic oscillators, one per site, with internal coordinates $\xi_{\mathbf{m}}$, frequency ω, and reduced mass M. The lattice is assumed to be infinite in all dimensions. The electron-phonon interaction is taken to be of the "density-displacement" form. No restriction is imposed on the form of *force* $f_{\mathbf{m}}(\mathbf{n})$ with which the electron at site $\mathbf{n}$ acts on $\mathbf{m}$th oscillator.

Since Feynman's classic work on polarons [15], it has been known that phonon degrees of freedom [variables $\vec{\xi}(\tau)$] can be integrated out in the path-integral representation of the partition function, Eq. (1), leading to a retarded self-interaction of the electron. For *periodic* BCIT, $\xi_{\mathbf{m}}(\beta) = \xi_{\mathbf{m}}(0)$, the phonon-induced part of the polaron action is [15]

$$A_{\mathrm{per}}[\mathbf{r}(\tau)] = \frac{\hbar}{4M\omega}\int_0^\beta\int_0^\beta d\tau_1\,d\tau_2\,\frac{\cosh\hbar\omega(\frac{\beta}{2} - |\tau_1 - \tau_2|)}{\sinh\frac{\hbar\omega\beta}{2}}\sum_{\mathbf{m}} f_{\mathbf{m}}(\mathbf{r}(\tau_1))f_{\mathbf{m}}(\mathbf{r}(\tau_2)), \tag{5}$$

where $\mathbf{r}(\tau)$ is the electron path. However, in the case of open BCIT the integration must be performed under the constraint $\xi_{\mathbf{m}+\Delta\mathbf{r}}(\beta) = \xi_{\mathbf{m}}(0)$, where $\Delta\mathbf{r} = \mathbf{r}(\beta) - \mathbf{r}(0)$ is the shift of the electron path. For nonzero $\Delta\mathbf{r}$ this yields an *extra term* in the action

$$\Delta A[\mathbf{r}(\tau)] = \frac{\hbar}{2M\omega}\sum_{\mathbf{m}} B_{\mathbf{m}}(C_{\mathbf{m}+\Delta\mathbf{r}} - C_{\mathbf{m}}), \tag{6}$$

where

$$B_{\mathbf{m}} = \int_0^\beta d\tau\, e^{-\hbar\omega\tau} f_{\mathbf{m}}(\mathbf{r}(\tau)), \qquad C_{\mathbf{m}} = \int_0^\beta d\tau\, e^{-\hbar\omega(\beta-\tau)} f_{\mathbf{m}}(\mathbf{r}(\tau)). \tag{7}$$

This formula is valid only in the limit $e^{\beta\hbar\omega} \gg 1$, which is easy to realize in practice. Thus, the integration over phonons reduces the problem to a single-particle system with an extra factor $\exp(A) = \exp(A_{\mathrm{per}} + \Delta A)$ in the weight of each path $\mathbf{r}(\tau)$.

I now describe how this factor should be incorporated into the general scheme of continuous-time QMC [16]. In d dimensions the hopping term in the Hamiltonian (4) introduces $2d$ *independent* Poisson processes with events, or "kinks" (after Ref. [2]), being jumps of an electron path to one of $2d$ nearest neighbors. The probability to have N_k kinks of a given sort on the time interval $[0, \beta]$ is given by the Poisson distribution $P_{N_k} = (N_k!)^{-1}(t\beta)^{N_k}e^{-t\beta}$. The Monte Carlo process consists of (i) proposing a change of the path by either removing existing kinks or adding new kinks and (ii) either accepting or rejecting the proposal. (Another possible subprocess is the shift of a kink in time but this can always be achieved by adding and removing.) Because of the open BCIT, it is sufficient to change the number of kinks just by one. When a kink is added (removed) at time τ_0 the *whole* path at $\tau > \tau_0$ is shifted in the corresponding direction (antidirection) by one lattice site (see Fig. 1). The balance equation for the adding-removing process is

$$q_a W(N_k)P_a(N_k \to N_k + 1) = q_r W(N_k + 1) \times P_r(N_k + 1 \to N_k), \tag{8}$$

where $W(N_k)$ is the probability to have a given path with N_k kinks of a given sort, and q_a and q_r are the probabilities of attempting to add or remove a kink, respectively. In this paper, $q_a = q_r = 1/2$ is used for $N_k \geq 1$, and $q_a = 1$, $q_r = 0$ for $N_k = 0$ (if there are no kinks of a given sort, one can only add one). In the absence of electron-phonon interaction the ratio $W(N_k + 1)/W(N_k) = t\beta/(N_k + 1)$ follows from the Poisson distribution. In the general case, each W is multiplied by its phonon-induced weight e^A. The acceptance rules now follow from Eq. (8):

$$P_a(N_k \to N_k + 1) = \min\left[1, \frac{t\beta}{N_k + 1}\,e^{A_{N_k+1} - A_{N_k}}\right], \tag{9}$$

to add a new kink to the existing N_k of a given sort, and

$$P_r(N_k + 1 \to N_k) = \min\left[1, \frac{N_k + 1}{t\beta}\,e^{A_{N_k} - A_{N_k+1}}\right], \tag{10}$$

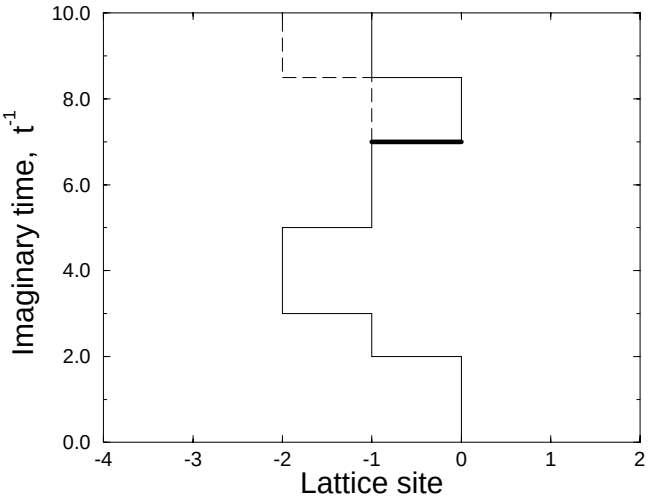

FIG. 1. A typical polaron path for $\beta = 10t^{-1}$ (solid line). When the kink at $\tau_0 = 7.0t^{-1}$ (bold line) is removed, the whole path at $\tau_0 < \tau < \beta$ is shifted to the left by one lattice site (dashed line). Δr changes from -1 to -2.

to remove one of the existing $N_k + 1$ kinks of a given sort. For the special case $N_k = 0$, the preexponential factor in Eq. (9) must be $t\beta/2$ instead of $t\beta$, and in Eq. (10) it must be $2/(t\beta)$ instead of $1/(t\beta)$.

The explicit form of the energy estimator that enters Eq. (2) follows from the $\Delta\tau \to 0$ limit of the corresponding finite-time expression [8]

$$-\frac{1}{w}\frac{\partial w}{\partial \beta} = -\frac{N_k^{\text{tot}}}{\beta} - \frac{\partial A}{\partial \beta}, \qquad (11)$$

where N_k^{tot} is the total number of kinks (of all sorts) on a path. Note that due to the open BCIT the thermodynamic estimator (11) measures the ground-state energy rather than full internal energy.

Summarizing the procedure, the QMC process samples single-particle paths with open BCIT by inserting and deleting kinks of $2d$ types. The acceptance rules for these two fundamental processes are given by Eqs. (9) and (10). The action A is a functional of the electron path $\mathbf{r}(\tau)$ and is given by the sum of Eqs. (5) and (6). Measured quantities include the energy estimator (11) and the inverse mass estimator $\frac{1}{\beta}[r_\alpha(\beta) - r_\alpha(0)]^2$. The polaron spectrum and effective mass are calculated with Eqs. (2) and (3), respectively. Note that statistics for *all* momenta (i.e., for as many **P** points as one wants) are collected during a *single* QMC run. In practical simulations successive measurements were taken every tenth single-kink step to reduce statistical correlations. For each set of model parameters several series of 500 000 or 1 000 000 measurements were conducted for different values of β to detect possible finite-temperature systematic errors, typically for $\beta\hbar\omega = 10$, 15, 20, and 25. No such errors were detected.

The method was tested on the Holstein model, for which independent numerical results are available. The Holstein model is a particular case of Eq. (4) with $f_{\mathbf{m}}(\mathbf{n}) = \kappa\delta_{\mathbf{mn}}$. The model is parametrized by the dimensionless frequency $\bar{\omega} = \hbar\omega/t$ and the dimensionless coupling constant $\lambda \equiv [\sum_{\mathbf{m}} f_{\mathbf{m}}^2(0)]/2dt\,M\omega^2 = \kappa^2/2dt\,M\omega^2$. Excellent agreement with previously published or communicated results was found. For example, in $d = 1$ [Figs. 2 and 3 (circles)] the present method's estimate of the ground-state energy for $\bar{\omega} = 1.0$, $\lambda = 0.5$ is $E_0 = -2.471 \pm 0.001$ (in units of t), with the true value being in the interval $(-2.46968, -2.471)$ [17]; for $\bar{\omega} = 1.0$, $\lambda = 1.0$ it yields $E_0 = -2.999 \pm 0.001$ with the true value in $(-2.99883, -3.000)$ [17]. For $\bar{\omega} = 1.0$ and $\lambda = 1.25$, 1.5, and 2.0, the estimated energies are -3.298, -3.623, and -4.388, respectively, which are, to within statistical error (± 0.002), precisely the values obtained by the exact diagonalization (ED) method [18]. For $\bar{\omega} = 2.0$ and $\lambda = 1.5625$ and 2.25, QMC yields $E_0 = -4.013$ and -5.070, respectively, in agreement with the strong-coupling perturbation theory [19]. Polaron masses obtained by QMC are in excellent agreement with variational calculations [17] and with density-matrix renormalization group (DMRG) results [11]. In $d = 2$, $\bar{\omega} = 1.0$ [Figs. 2 and 3 (filled squares)], QMC's energies agree with ED [20] and QMC's masses agree with DMRG [11]. All of these checks confirm that the present algorithm is free from systematic errors of any kind. Statistical errors are small, 0.1%–0.3% in most cases.

As a new application of the method the ground-state energy and effective polaron mass were calculated for the three-dimensional Holstein model [see Figs. 2 and 3 (triangles)]. At present, three-dimensional lattices are out of reach of ED and DMRG methods due to the enormous phonon Hilbert space. The present Monte Carlo algorithm treats all of the phonons in an infinite lattice exactly through the analytical integration so the lattice size is irrelevant. Another advantage of the method is its ability to study long-range electron-phonon interactions. Indeed,

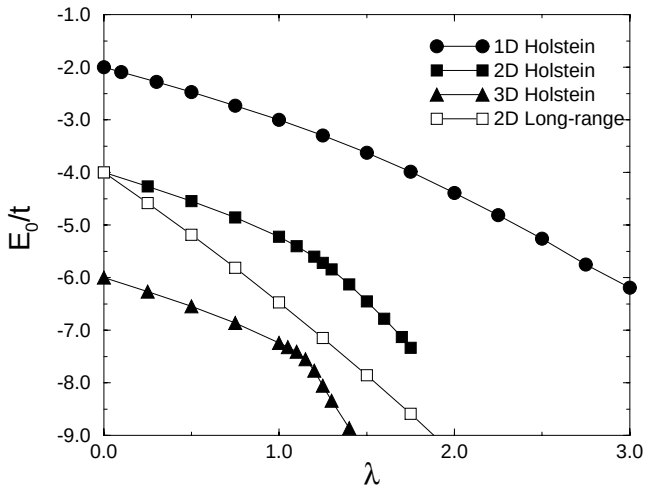

FIG. 2. Ground-state polaron energy for several models. In all cases, $\bar{\omega} = 1.0$. Statistical errors are smaller than the symbols.

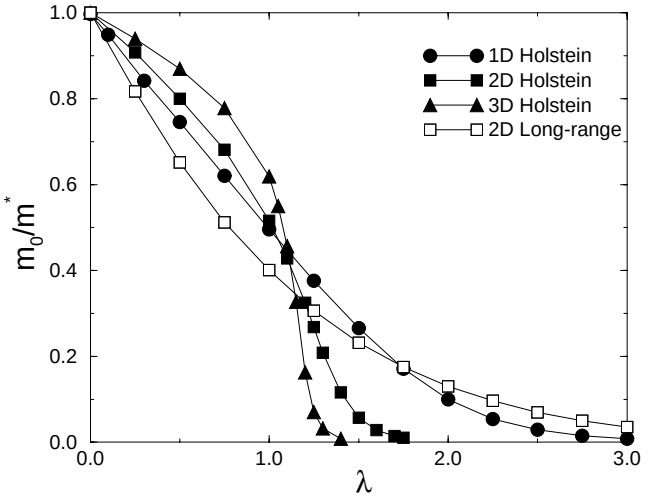

FIG. 3. Inverse effective polaron mass in units of $1/m_0 = 2ta^2/\hbar^2$ for several models. In all cases, $\bar{\omega} = 1.0$. Statistical errors are smaller than the symbols.

the interaction enters the formalism only via lattice sums $\sum_{\mathbf{m}} f_{\mathbf{m}}(\mathbf{r}_1) f_{\mathbf{m}}(\mathbf{r}_2)$ which can be computed in advance for all $\mathbf{r}_1 - \mathbf{r}_2$ and stored for later calculation of the action A. Figures 2 and 3 (open squares) show results for $f_{\mathbf{m}}(\mathbf{n}) = \kappa(|\mathbf{m} - \mathbf{n}|^2 + 1)^{-3/2}$ in $d = 2$ (for this interaction, $\lambda = 1.742\kappa^2/4tM\omega^2$). This form of $f_{\mathbf{m}}(\mathbf{n})$ has recently been proposed to model the interaction between in-plane holes and *apical* oxygens in high-T_c superconductors [21]. One can see that at large λ the polaron is much lighter than in the Holstein case. Indeed, a long-range interaction results in "wider" polaron paths and, consequently, in a smaller effective mass by virtue of Eq. (3). Finally, I present the polaron *spectrum* in the $d = 1$ Holstein model for $\bar{\omega} = 1.0$ and $\lambda = 1.75$, calculated with Eq. (2) (see Fig. 4). The spectrum flattens at large momenta as was revealed in previous numerical studies [22,23]. The actual energies

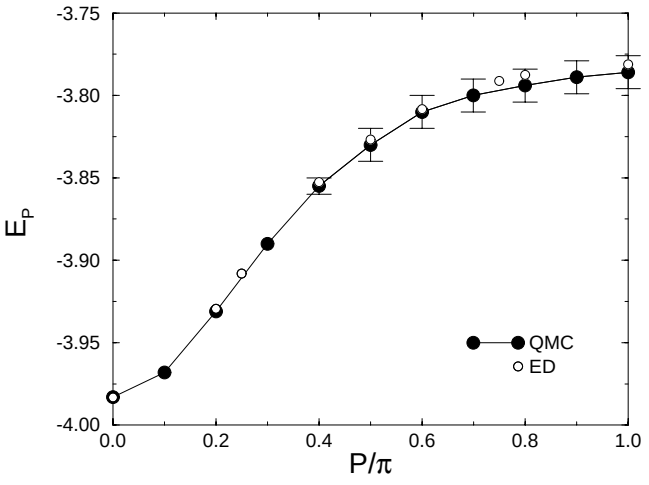

FIG. 4. The polaron spectrum E_P (in units of t) in the one-dimensional Holstein model for $\bar{\omega} = 1.0$ and $\lambda = 1.75$. Open circles are exact diagonalization results [20].

E_P are in excellent agreement with ED results [20]. This demonstrates that a *real-time* spectrum can be measured directly by an *imaginary-time* path-integral QMC.

In conclusion, an efficient continuous-time path-integral quantum Monte Carlo algorithm for the lattice polaron has been presented. It is free from the finite-size and finite-time-step systematic errors. The method works for infinite lattices and any range of electron-phonon interaction. It allows for exact calculation of the ground-state energy, effective mass, and spectrum of the polaron. More technical details will be presented elsewhere.

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[1] H. De Raedt and A. Lagendijk, Phys. Rep. **127**, 233 (1985).
[2] N. V. Prokof'ev, B. V. Svistunov, and I. S. Tupitsin, JETP Lett. **64**, 911 (1996).
[3] B. B. Beard and U.-J. Wiese, Phys. Rev. Lett. **77**, 5130 (1996).
[4] V. A. Kashurnikov *et al.*, cond-mat/9802294 [Phys. Rev. B (to be published)].
[5] B. Ammon *et al.*, Phys. Rev. B **58**, 4304 (1998).
[6] V. A. Kashurnikov, A. V. Krasavin, and B. V. Svistunov, Phys. Rev. B **58**, 1826 (1998).
[7] N. V. Prokof'ev and B. V. Svistunov, Phys. Rev. Lett. **81**, 2514 (1998).
[8] H. De Raedt and A. Lagendijk, Phys. Rev. Lett. **49**, 1522 (1982); Phys. Rev. B **27**, 6097 (1983).
[9] A. S. Alexandrov, V. V. Kabanov, and D. K. Ray, Phys. Rev. B **49**, 9915 (1994), and references therein.
[10] H. Fehske, J. Loos, and G. Wellein, Z. Phys. B **104**, 619 (1997), and references therein.
[11] E. Jeckelmann and S. R. White, Phys. Rev. B **57**, 6376 (1998).
[12] P. E. Kornilovitch and E. R. Pike, Phys. Rev. B **55**, 8634 (1997).
[13] C. Alexandrou and R. Rosenfelder, Phys. Rep. **215**, 1 (1992), and references therein.
[14] M. Boninsegni and D. M. Ceperley, Phys. Rev. Lett. **74**, 2288 (1995).
[15] R. P. Feynman, Phys. Rev. **97**, 660 (1955); *Statistical Mechanics* (Benjamin, Reading, 1972).
[16] N. V. Prokof'ev, B. V. Svistunov, and I. S. Tupitsin, Sov. Phys. JETP **87**, 310 (1998).
[17] A. H. Romero, D. W. Brown, and K. Lindenberg, cond-mat/9710321.
[18] V. V. Kabanov (private communication).
[19] W. Stephan (private communication).
[20] G. Wellein and H. Fehske (private communication).
[21] A. S. Alexandrov and P. E. Kornilovitch, cond-mat/9808198.
[22] G. Wellein, H. Röder, and H. Fehske, Phys. Rev. B **53**, 9666 (1996).
[23] W. Stephan, Phys. Rev. B **54**, 8981 (1996).