Path-integral method for a heavy particle moving in a periodic potential and screened by a light degenerate Fermi gas

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We study a heavy particle moving in a periodic lattice of arbitrary dimension and interacting with a degenerate fermionic heat bath. We assume that the Fermi energy of the screening particles is large compared to the tight-binding bandwidth of the particle. We develop a path-integral method for the partition function of the heavy particle where we integrate out the electronic degrees of freedom. We perform also a summation over the paths between the screening-interaction points that makes the method capable of treating band motion and hopping. Following the method of Anderson and Yuval, we derive scaling equations by eliminating that part of the phase space of the light particles which is far from the Fermi energy. We find that the screening strength is not renormalized; the bandwidth of the heavy particle is, however, essentially reduced. That reduction coincides with the reduction in the two-site model. Extrapolating the result for larger values of the screening strength we find band motion and localization at zero temperature depending on the coupling strength; thus the behavior is of Ohmic type. We show that the results obtained can be combined with the classical kinetic equation to get the diffusion coefficient. We believe that the present work based on the path-integral method helps to clarify the connection between results obtained by different methods. The relation of the model to other models, especially to the Caldeira-Leggett model, is discussed in detail.

I. INTRODUCTION

In the last several years, the problem of the motion of a heavy particle interacting with a light degenerate Fermi gas has attracted considerable interest.[1] That problem has many important implications for, for example, the diffusion of muons or hydrogen in metals, the motion of heavy ions in the degenerate Fermi liquid ^{3}He, the mass reduction of heavy d electrons in transition metals, and very likely heavy-fermion systems. The problem has been attacked by different methods: first, the direct perturbation theory and summation of diagrams in the logarithmic approximation by Kondo and Soda[2] and then the generalization of this method developed by Kagan and coworkers[3,4] for the small-polaron problem, which is combined with the kinetic equation. This problem has also a strong resemblance to the Caldeira-Leggett[5,6] problem, where a moving particle is coupled to a heat bath with many degrees of freedom. The latter has been almost exclusively treated by the path-integral method. The present paper is devoted to developing a path-integral treatment for a particle moving by hopping on a lattice and coupled to a degenerate Fermi gas. We believe that the present method helps to make the relationship between the different methods more transparent; furthermore it establishes a stronger connection to a similar problem where the hopping motion is restricted to only two sites, known as the two-level system (TLS).[6,8] Finally, we suggest that the present method is applicable to heavy-fermion systems as well. In the following we give a brief discussion of the methods that have been already developed.

The common features of all of the many-site systems are that the screening by the light particles results in the reduction of the hopping rate or of the bandwidth of the heavy particles, and that the interaction between the heavy and light particles is not renormalized. Furthermore, in the case of the hopping model for the heavy particle, the light-particle-assisted hopping or tunneling,[7] also called incoherent hopping, is not included. We know that the assisted tunneling changes the behavior of the two-site problem in an essential way;[7] however, it will not be included in the present paper either. In general, the renormalizations of the parameters of the heavy particle are due to Anderson's orthogonality catastrophe,[9] namely, at zero temperature, $T=0$, the screening clouds formed by the light particles around the heavy ones placed at two different sites are orthogonal to each other. At zero temperature, if the coupling is strong enough, the heavy particle is localized; in other words, its mass diverges and the hopping matrix element Δ behaves like

$$\Delta(T)=\Delta_0\left[\frac{T}{D}\right]^K \quad \text{for } K>1 \ , \tag{1.1}$$

where Δ_0 is the unrenormalized hopping rate, D is the light-particle bandwidth, and K is proportional to the square of the coupling responsible for the screening. In

the case of weak coupling, $K<1$, the above renormalization provides a reduction of the hopping rate as the temperature is lowered, but the renormalization saturates as the temperature becomes comparable to the hopping rate. In that case, the smallest value of the hopping rate Δ_c is the solution of the equation

$$\Delta_c=\Delta_0\left[\frac{\Delta_c}{D}\right]^K \quad \text{for } K<1 \ . \tag{1.2}$$

In the following two approaches either the band or the hopping motion of the heavy particle is emphasized. In the band picture, Kondo and Soda[2] attacked the problem by using perturbation theory, and they showed that the heavy-particle self-energy has a logarithmic correction in the second order in the perturbation theory. The argument of the logarithm is the temperature or the energy of the heavy particle divided by the band cutoff of the degenerate Fermi gas, which is of the order of the Fermi energy. By summing a certain class of diagrams, the results given by expressions (1.1) and (1.2) can be obtained.[10] These renormalizations must be taken into account in the kinetic equations, as recently justified by Yamada[11] in the framework of the Green's-function technique. The solution of those equations gives the mobility and the diffusion constant in agreement with the results based on the Kubo formula.[12] At finite temperature the diffusion is limited by the creation of light particle-hole pairs, and the diffusion constant shows a power behavior in its temperature dependence.

There is another approach to the problem which was first suggested by Kagan and Klinger[3] for the small-polaron problem. In that method first the hopping rate to a neighboring site is determined, which means a calculation of the overlap integral of the two screening clouds. Such calculations have been recently performed in great detail.[13–16] The second step is to build the hopping rate obtained into a kinetic equation[3] for the heavy particle where the variables of the light particles are integrated out.[3,4] Such a program has been performed by Kagan and Prokof'ev[17] and by Yamada *et al.*[15]

Considering the theory of Caldeira and Leggett,[5] the most interesting are those models in which the dissipation of the motion of the heavy particle due to the light ones is of Ohmic type. The condition for Ohmic dissipation was given by Kagan and Prokof'ev[17] in terms of a function $f(\omega)$ defined as

$$f(\omega)=\sum_\alpha \frac{|C_\alpha^{(i)}-C_\alpha^{(j)}|^2}{\omega_\alpha}\delta(\omega-\omega_\alpha) \ , \tag{1.3}$$

where ω_α stands for the energy of different excitations in the heat bath and $C_\alpha^{(i)}$ is the coefficient in the interaction Hamiltonian in front of the product of creation and annihilation operators obeying the usual Bose or Fermi commutation rules, assuming that the heavy particle is at site i. The system shows Ohmic behavior if $\lim_{\omega\to 0}f(\omega)=$const for $i\neq j$. That is the marginal case, where we have different behavior for $K>K_c$ and $K<K_c$ as shown by Eqs. (1.1) and (1.2) with $K_c=1$. If $\lim_{\omega\to 0}f(\omega)=0$ or ∞ then we always have a delocalized or a localized state, respectively, at $T=0$.

In the case of a bosonic and of a fermionic heat bath the constant $C_\alpha^{(i)}$ contains a phase factor $e^{iq_\alpha R_i}$ where R_i is the position of the heavy particle and q_α is the total momentum of the excitation in the heat bath. That phase factor is not introduced explicitly in the Caldeira-Leggett model.[5,18–20] The source of a further formal difference is that the latter authors introduce the coupling $F(R)$ in the interaction Hamiltonian $\sum_\alpha F_\alpha(R)x_\alpha$ where R and x_α are the coordinates of the heavy particle and the oscillator, respectively.

Considering Eq. (1.3), the condition for Ohmic behavior depends on the dimensionality d of the system. In the case $d=1$ we must distinguish between models where the electron scattering is forward or backward. In case of forward scattering, the momentum transfer q_α is small, $C_\alpha^{(i)}\sim e^{iq_\alpha R_i}$, $\omega_\alpha\sim q_\alpha$, and the density of the electron-hole excitations is proportional to ω: thus, $f(\omega)\sim\omega^2$ for small ω. In the case of backscattering, the momentum transfer is $q\sim 2k_F$, where k_F is the Fermi momentum; thus $f(\omega)\to$const as $\omega\to 0$ and we find Ohmic behavior. Recently, Itai[21] has treated the forward-scattering model by transforming the electron density operators into Tomonaga bosons. In the case $d>1$ the momentum transfer is large (q connects two arbitrary points of the Fermi surface), thus those models always exhibit Ohmic behavior.

Finally, we comment on the Caldeira-Leggett[5] model where $F_\alpha(R)\sim R$, in which case their well-known expression for the friction coefficient holds. That model has been used also for one-dimensional (1D) diffusion by Schmid[18] and several other authors.[19,20] As has recently been pointed out by Zawadowski[22] and Itai[21] the hopping models of Schmid's type can be derived only in the localized region by expanding the factor $e^{iq_\alpha R_i}\sim 1+iq_\alpha R_i$, where an extra factor of q_α occurs. In order to compensate for that extra factor the coupling to acoustic phonons with a constant density of states must be modified to $C_\alpha^{(i)}\sim q_\alpha^{-1/2}e^{iq_\alpha R_i}$ in contrast to the physical coupling to longitudinal phonons where $C_\alpha^{(i)}\sim q^{1/2}e^{iq_\alpha R_i}$. Thus, Schmid's 1D theory is valid for a special coupling in the localized region where $qR_i\ll 1$ holds for the infrared processes and for the dynamics of superconducting quantum-interference devices.

In the path-integral method two different couplings for the hopping of the heavy particle, Δ, and the screening strength must be taken into account. One gets a partition function of a simpler form if the summation in one of those couplings is carried out explicitly. Itai[21] was able to perform that summation for the forward scattering of electrons, and in case, e.g., of the Kondo problem[23,24] or of TLS's[8,25,26], the contribution of the electronic screening can be summed up by solving the Noziéres–de Dominicis equation for the electron Green's function. In the present problem that solution would be needed for the time- and space-dependent external potential representing the heavy particle. We were not able to solve that problem. We performed the summation, however, for the hopping between the screening-interaction points using a result of Coleman[27] where he introduces the tight-binding band structure for the heavy particle. In this way in our calculation we do not need to differentiate between hopping and band motions.

In the present paper we treat the case of large momentum transfer in arbitrary dimension d (the backscattering model in 1D. We consider an arbitrary hopping path of the heavy particle on a lattice, where the path is decorated by the interaction points. As a first step we write the partition function in the form proposed by Yuval and Anderson[23] in the Kondo problem where the screening points, e.g., τ_i and τ_j on the imaginary time axis interact by a logarithmic interaction $\ln|\tau_i-\tau_j|$. Then we perform the summation over all possible paths between the screening-interaction points shown in Fig. 1. In the expression of the partition function we are not able to perform the explicit summation over the directions of the electrons, therefore we use the scaling method developed by us[26] where the scaling is established in the individual terms. Using the Anderson, Yuval, and Hamann method,[24] we derive the scaling eliminating the short-time behavior (close screening-interaction points), and compensating for that by renormalizing the overlap integral Δ and the screening couplings. The latter turns out to be actually invariant. Finally, we discuss the fact that the renormalized overlap integral Δ can be used in the classical kinetic equation to get the diffusion coefficient at finite temperature.

In Sec. II the model is formulated and the form of the electron Green's function is discussed. In Sec. III the form of the partition function is derived in the 1D case. Section IV is devoted to the derivation of the scaling equation and the results with their discussions are presented in Sec. V.

II. FORMULATION OF THE MODEL

We consider a particle moving by hopping on a lattice, coupled to a degenerate Fermi gas in arbitrary dimension d. The Hamiltonian takes the form

$$H=H_0+H_{11}+H_{12}\ , \tag{2.1}$$

where

$$H_0=v_F\sum_{\mathbf{k},s}(|\mathbf{k}|-k_F)a^\dagger_{\mathbf{k}s}a_{\mathbf{k}s}\ , \tag{2.2}$$

$$H_{11}=\Delta\sum_{n,\delta}c^\dagger_{n+\delta}c_n\ , \tag{2.3}$$

$$H_{12}=\frac{1}{L^d}\sum_n\sum_{\mathbf{k},\mathbf{k}',s}V_{\mathbf{k}\mathbf{k}'}c^\dagger_n c_n a^\dagger_{\mathbf{k}s}a_{\mathbf{k}'s}e^{i(\mathbf{k}'-\mathbf{k})\cdot\mathbf{R}_n}\ . \tag{2.4}$$

Here L is the size of the sample, v_F and k_F are the Fermi velocity and momentum, respectively, and we apply a momentum cutoff $-D<v_F(|\mathbf{k}|-k_F)<D$, where D is of the order of the electron bandwidth. We take a constant density of state for the electrons. The creation and annihilation operators of the electrons with momentum $\mathbf{k}$ and spin s are $a^\dagger_{\mathbf{k}s}$ and $a_{\mathbf{k}s}$. The c_n and $c^\dagger_n$ operators destroy and create the particle at the well labeled by n at position $\mathbf{R}_n$ and $n+\delta$ labels the positions $\mathbf{R}_{n+\delta}$ which are the nearest neighbors of position $\mathbf{R}_n$. Δ is the hopping amplitude for the particle and $V_{\mathbf{k}\mathbf{k}'}$ is the interaction matrix element.

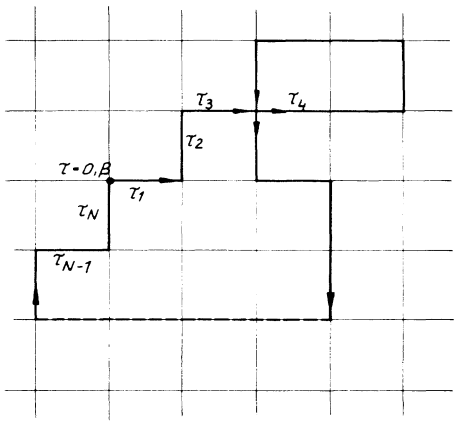

FIG. 1. Typical hopping path on a two-dimensional lattice is depicted. The path starts and ends at the same lattice point labeled by 0. The time τ_i $(i=1,\ldots,N)$ of the ith hop is also indicated. The dashed line represents an arbitrary path connecting the end points.

We calculate the partition function of the system by using the imaginary-time technique and the functional-integral approach for the particle. The functional integral in the expression of the partition function,

$$Z=\int D\mathbf{R}Z_I(\mathbf{R}(\tau))\ , \tag{2.5}$$

is taken over all the possible hopping paths $\mathbf{R}(\tau)$ on the lattice (see Fig. 1) and the partition function $Z_I(\mathbf{R}(\tau))$ is given in the interaction representation with respect to H_0 as

$$Z_I=\mathrm{Tr}\left[e^{-\beta H_0}T_\tau\exp\left[-\int_0^\beta d\tau H_1(\tau)\right]\right]\ , \tag{2.6}$$

where T_τ is the imaginary-time–ordering operator, β is the inverse temperature, and the trace is taken over the electron states. In the following, we will use the low-temperature approximation of Anderson *et al.*[24] and Hamann,[28] where the trace is replaced by the ground-state expectation value denoted by $\langle\ \rangle$. As pointed out by those authors, the results obtained in that approximation can be generalized to finite temperatures by straightforward modifications to their final form. For a given path with N_y hopping steps (with hopping fugacity y) and with N_v electron-particle interactions $(N=N_y+N_v)$ we obtain Z_{N_y,N_v} by expanding the exponential in Eq. (2.6) as

$$\begin{aligned}Z_{N_y,N_v}&=\sum_{\{\alpha\}}(-1)^N\int_0^\beta d\tau_N\cdots\int_0^{\tau_{i+1}}d\tau_i\cdots\int_0^{\tau_2}d\tau_1\langle S(\beta,\tau_N)H_{1\alpha_N}S(\tau_N,\tau_{N-1})\cdots H_{1\alpha_1}S(\tau_1,0)\rangle\\&=\sum_{\{\alpha\}}L^{-dN_v}\sum_{\{\mathbf{k},\mathbf{k}'\}}\sum_{\{s\}}(-1)^{N_y+N_v}\int_0^\beta d\tau_N\cdots\int_0^{\tau_{i+1}}d\tau_i\cdots\int_0^{\tau_2}d\tau_1\Delta^{N_y}\\&\quad\times\left\langle T_\tau\left[\prod_i{}^{(s)}V_{\mathbf{k}_i\mathbf{k}_i'}a^\dagger_{\mathbf{k}_i s_i}(\tau_i)a_{\mathbf{k}_i' s_i}(\tau_i)e^{i(\mathbf{k}'-\mathbf{k})\cdot\mathbf{R}_n}\right]\right\rangle\left\langle n_0\left|\prod_i(c^\dagger_{n_i}c_{n_i'})\right|n_0\right\rangle\ ,\end{aligned} \tag{2.7}$$

where $S(\tau,\tau')$ is the time-evolution operator due to H_0, n_i (n_i') labels the position of the particle immediately after (before) the interaction process labeled by i, and, formally, the c_n operators are kept to indicate the path with coinciding initial and final state $|n_0\rangle$. The index α_i of the interaction $H_{1\alpha_i}$ has two values $\alpha_i=1,2$ and the summation covers all of the possible configurations $\{\alpha\}=(\alpha_1,\alpha_2,\ldots,\alpha_N)$. The momentum integrals are represented by summation over the momenta of all of the possible electron creation and annihilation operator pairings in the momentum interval $-D<(|\mathbf{k}|-k_F)v_F<D$, which are denoted briefly by the configuration $\{\mathbf{k},\mathbf{k}'\}$, and $\{s\}$ is a similar configuration for the electron spins s_i. Furthermore, $\prod^{(s)}$ means the product associated with the electron-particle scatterings described by the Hamiltonian H_{12}. Finally, the boundary condition for the paths $\mathbf{R}_n(\tau)$ is $n(0)=n(\beta)=n_0$, which is an arbitrary position.

Next we evaluate the expectation value in Eq. (2.7) with the help of Wick's theorem. In course of this, we have to consider all possible pairings of the operators $a_{\mathbf{k}}$ and $a_{\mathbf{k}'}^{\dagger}$ where the pairings are associated with the Green's functions $G^{(0)}(\tau,\tau';\mathbf{k})$ to be determined next.

The following treatment is based on the approximation that the interaction strength $V_{\mathbf{k}\mathbf{k}'}$ depends only on the directions $\hat{\boldsymbol{\kappa}}=\mathbf{k}/|\mathbf{k}|$ and $\hat{\boldsymbol{\kappa}}'=\mathbf{k}'/|\mathbf{k}'|$ but does not depend on the absolute values $|\mathbf{k}|$ and $|\mathbf{k}'|$. Thus the summations over the absolute values of the momenta can be performed for each Green's function separately, and we obtain a mixed real-space–momentum-direction representation in which the Green's function is

$$G^{(0)}(\tau-\tau';\mathbf{R}-\mathbf{R}',\hat{\boldsymbol{\kappa}})=\frac{1}{L}\sum_{|\mathbf{k}|}e^{-\varepsilon_k(\tau-\tau')}e^{i\mathbf{k}\cdot(\mathbf{R}-\mathbf{R}')}[n_F(\varepsilon_k)-\Theta(\tau-\tau')]$$
$$=e^{ik_F(\mathbf{R}-\mathbf{R}')\cdot\hat{\boldsymbol{\kappa}}}\int_{-D}^{D}\rho\,d\varepsilon\,e^{-\varepsilon(\tau-\tau')}e^{i\varepsilon v_F^{-1}(\mathbf{R}-\mathbf{R}')\cdot\hat{\boldsymbol{\kappa}}}[n_F(\varepsilon_k)-\Theta(\tau-\tau')]\ , \tag{2.8}$$

where $\varepsilon_k=v_F(k-k_F)$ is the electron energy, ρ stands for the electron density of state for a given direction n, $n_F(\varepsilon)$ is the Fermi distribution function, and $\Theta(\tau)$ is the step function [$\Theta(\tau)=1$ for $\tau>0$ and $\Theta(\tau)=0$ for $\tau<0$]. In the region $\tau_0=D^{-1}\ll|\tau-\tau'|\ll\beta$, the bare Green's function is obtained by evaluating the integral in Eq. (2.8), thus

$$G_s^{(0)}(\tau-\tau';\mathbf{R}-\mathbf{R}',\hat{\boldsymbol{\kappa}})$$
$$=e^{ik_F(\mathbf{R}-\mathbf{R}')\cdot\hat{\boldsymbol{\kappa}}}\frac{\rho}{\tau'-\tau+i(\mathbf{R}-\mathbf{R}')\cdot\hat{\boldsymbol{\kappa}}v_F^{-1}} \tag{2.9}$$

for $|\tau-\tau'|D\gg1$. The averaged distance $|\mathbf{R}-\mathbf{R}'|$ covered by the particle during the time interval $|\tau-\tau'|$ is $|\mathbf{R}-\mathbf{R}'|\lesssim|\tau-\tau'|b\Delta$, where b is the lattice spacing. Furthermore, we assume that $\Delta\ll\varepsilon_F$, thus the following inequality holds:

$$|\mathbf{R}-\mathbf{R}'|\ll b|\tau-\tau'|\varepsilon_F\sim|\tau-\tau'|v_F\ , \tag{2.10}$$

and therefore we will approximate the Green's function given by Eq. (2.8) as

$$G_s^{(0)}(\tau-\tau';\mathbf{R}-\mathbf{R}',\hat{\boldsymbol{\kappa}})=e^{ik_F(\mathbf{R}-\mathbf{R}')\cdot\hat{\boldsymbol{\kappa}}}\frac{\rho}{\tau'-\tau}\ . \tag{2.11}$$

In the path-integral method there are, however, paths where the hops are much closer than Δ^{-1}. The argument presented here clearly shows that expression (2.11) holds assuming that the time difference between hops is larger than a characteristic time $\tau_0\geq\varepsilon_F^{-1}$. That time τ_0 will be related to the short-time cutoff which we will discuss in Sec. V in more detail.

We will first evaluate the partition function in the case of one dimension with backscattering. The generalization for higher dimensions will be given in Sec. III.

III. PARTITION FUNCTION AND SCALING IN THE ONE-DIMENSIONAL CASE

The formulas are shorter for the one-dimensional model with backscattering only; therefore, we give the detailed calculation for that case. The direction of the momentum $\hat{\boldsymbol{\kappa}}$ has only two values $\mu=\pm1$, thus the Green's function given by Eq. (2.11) has two forms for $\mu=\pm1$:

$$G_{s\mu}^{(0)}(\tau-\tau';n-n')=\frac{\rho}{\tau-\tau'}e^{i\mu Q(n-n')}\ , \tag{3.1}$$

where $Q=k_Fb$ is the dimensionless Fermi momentum and n corresponds to the site at R_n. The left- and right-hand sides of the one-dimensional electron dispersion curve contribute to $G_{s-}^{(0)}$ and $G_{s+}^{(0)}$, respectively. Furthermore, the backscattering electron-particle coupling $V_{\mathbf{k}\mathbf{k}'}$ becomes a single number V. First we give an expression for the partition function and then we establish the scaling in terms of the cutoff.

A. Partition function

The ground-state expectation value on the right-hand side (rhs) of Eq. (2.7) can be evaluated directly by carrying out the integrals with respect to the absolute values of the momenta, and then we introduce the Green's functions of the form given by Eq. (2.11). We closely follow the method developed by Yuval and Anderson[23] and used by the present authors[26] where the sum of the contributions of different pairings in the evaluation of the expectation value is a product of determinants of Cauchy type. We determine the ground-state expectation value in Eq. (2.7) in that way. The summation over the momentum configurations $\{\mathbf{k},\mathbf{k}'\}$ is carried out in two steps. First we introduce the configuration $\{\mu\mu'\}$ which gives the directions of the momenta of the outgoing and ingoing electrons at each interaction point i. As $\mu_i=-\mu_i'$ holds for

backscattering, therefore we can introduce the simpler notation $\{\mu\}=\{\mu\mu'\}$. The summations remaining to be carried out are restricted for given sides of the dispersion curve $k_i \gtrless 0$ and $k_i' \lesseqgtr 0$, which are determined by the configuration $\{\mu\}$ but must include all the possible pairings allowed by the configuration $\{\mu\}$. Thus we can give the expectation value occurring in Eq. (2.7) for a given configuration $\{\mu\}$ as

$$\left\langle T_\tau \prod_i^{(s)} \sum_{k_i,k_i'} a^\dagger_{k_i s_i}(\tau_i) a_{k_i' s_i}(\tau_i) e^{i(k_i'-k_i)R_i} \right\rangle$$
$$= R \prod_{s,\mu=\pm 1} R_{s\mu} \left[\sum_P (-1)^{p(P)} \prod_i^{(s)} G^{(0)}_{s\mu}(\tau_{\lambda_i^{s\mu}}, \tau_{\eta^{s\mu}_{P(i)}}) \right]$$
$$= R \exp\left[-2iQ \sum_i \mu_i n_i \right] \prod_{s,\mu=\pm 1} R_{s\mu} \det_{s\mu} \left[\frac{\rho}{\tau_j - \tau_i} \right] . \tag{3.2}$$

We have obtained the expression above in the following way.[26] First we have written the expectation value as a product corresponding to electron operators with different (s,μ) index pairs.

The indices $\lambda_i^{s\mu}$ ($\eta_i^{s\mu}$) are those subseries of the interaction indices $i=1,\ldots,N_s$ for which the creation (annihilation) operators have common index pairs (s,μ). R and $R_{s\mu}$ are combinational factors $R=(-1)^{\tilde{P}}$ where $\tilde{P}$ is the number of those neighbor exchanges in the product of the creation and annihilation operators which are required to group the operators with respect to the index pairs (s,μ) by exchanging operators only with different (s,μ) indices. Furthermore, $R_{s\mu}=(-1)^{P_{s\mu}}$, where $P_{s\mu}$ is the number of the further neighbor exchanges in the group characterized by the index pair (s,μ) in order to get an alternative sequence of annihilation and creation operators by exchanging creation operators only with annihilation operators. Then we apply the Wick's theorem for those groups of operators. Considering the alternative sequence of annihilation and creation operator in group (s,μ) any possible pairings can be associated with permutation $P(i)$ of the $\eta_i^{s\mu}$ indices, where the original ith index is changed to $\eta^{s\mu}_{P(i)}$ in the new series. Furthermore, the parity of permutation $P(i)$ is $p(P)=0$ or 1. The determinant $\det_{s\mu}$ is defined only for those indices i and j which are associated with operators belonging to the group (s,μ). The parity $p(P)$ is contained in the definition of a determinant. The determinant is known as the Cauchy determinant[29] which has the value

$$\det\left[\frac{1}{\tau_i-\tau_j}\right] = \frac{\prod_{i,i'\ (i<i')} (\tau_i-\tau_{i'}) \prod_{j,j'\ (j>j')} (\tau_j-\tau_{j'})}{\prod_{i,j} (\tau_i-\tau_j)} ; \tag{3.3}$$

considering the determinant $\det_{s\mu}$, the inequality $\tau_i \neq \tau_j$ holds as only backscattering is considered. The final form for the expression in Eq. (3.2) can be written in a compact form by introducing charges as in Refs. 25 and 26. In the present case $T^i_{s\mu}$ is defined for the interaction point i as

$$T^i_{s\mu} = \begin{cases} +1 & \text{if only the outgoing electron line has the label } (s,\mu), \\ -1 & \text{if only the ingoing electron line has the label } (s,\mu), \\ 0 & \text{otherwise .} \end{cases} \tag{3.4}$$

Using Eq. (3.3) and definition (3.4) we get for the expectation value in Eq. (3.2)

$$\langle \cdots \rangle = R \exp\left[-i2Q \sum_i \mu_i n_i \right] \times \prod_{s,\mu} \left[(\rho\tau_0^{-1})^{N_{s\mu}} \prod_{i,j\ (i<j)} \left| \frac{\tau_i-\tau_j}{\tau_0} \right|^{T^i_{s\mu}T^j_{s\mu}} \right] , \tag{3.5}$$

where $N_{s\mu}$ is the order of the determinant $\det_{s\mu}$ and the factor $R_{s\mu}$ is taken into account by taking the absolute values; furthermore, the cutoff time τ_0 to be defined later is introduced for further convenience.

By combining the expressions (3.2), (3.4), and (3.5) with Eq. (2.7) we can give the contribution Z_{N_y,N_v} of a given path decorated by the electron-particle interaction in the following form:

$$Z_{N_y,N_v} = \sum_{|\alpha|} \sum_{\{\mu\},\{s\}} (-1)^N R \int_0^\beta d\tau_N \cdots \int_0^{\tau_{i+1}} d\tau_i \cdots \int_0^{\tau_2} d\tau_1 \tau_0^{-N} y^{N_y} v^{N_v} \times \exp\left[-i2Q \sum_i n_i\mu_i + \sum_{s,\mu} \sum_{i,j\ (i<j)} T^i_{s\mu}T^j_{s\mu} \ln\frac{|\tau_i-\tau_j|}{\tau_0} \right] \left\langle n_0 \left| \prod_i (c^\dagger_{n_i} c_{n_i'}) \right| n_0 \right\rangle , \tag{3.6}$$

where we took the summations over the configuration $\{\mu\}$ of the momentum directions and we introduced the dimensionless hopping transition fugacities y and electron scattering amplitudes v as

$$y = \Delta\tau_0 , \tag{3.7}$$

where

$$v = V\rho . \tag{3.8}$$

Finally, we mention that the short-time cutoff introduced by Yuval and Anderson[23] for minimal time difference between interactions will be introduced later.

B. Summation over the hopping transitions

The hopping transitions and electron scatterings are the interaction points occurring in the expression for the free energy Z_{N_v,N_v} given by Eq. (3.6). In that expression the summation with respect to the hopping transitions can be carried out by inserting an arbitrary number of hopping transitions between the electron-particle scatterings. That we can do easily as the charges for the hoppings $T^i_\mu=0$, thus they do not interact by logarithmic interaction.

We consider an arbitrary path with N_s electron scattering processes occurring at times τ_i and places n_i. We take now two successive electron scattering processes at time points τ_i and τ_j $(\tau_i<\tau_j)$ at positions n_i and n_j, respectively. Then we inset m hopping transitions to the right and m' to the left assuming that $m-m'=n_j-n_i$. The corresponding particle transition operator is

$$c^\dagger_{n_j}c_{n_i}\sum_{m,m'=0}^{\infty}(-1)^{m+m'}\delta_{(n_j-n_i),(m-m')} \times\frac{1}{m!m'!}y^{m+m'}\tau_0^{-(m+m')}(\tau_j-\tau_i)^{m+m'}\ , \quad (3.9)$$

where δ stands for the Kronecker symbol and we assumed that the hopping transitions can be placed with an arbitrarily small time difference. That point will be discussed later.

The summations over m and m' can be performed; following Coleman[27] we use the integral representation of the Kronecker symbol

$$\delta_{(n_j-n_i),(m-m')}=\int_{-\pi}^{\pi}\frac{d\theta}{2\pi}e^{i\theta[(n_j-n_i)-(m-m')]}\ . \quad (3.10)$$

By combining expression (3.9) with Eq. (3.10) we get

$$(-1)^{n_j-n_i}c^\dagger_{n_j}c_{n_i}\int_{-\pi}^{\pi}\frac{d\theta}{2\pi}e^{i\theta(n_j-n_i)} \times\exp\left[2y\frac{(\tau_j-\tau_i)}{\tau_0}\cos\theta\right]\ . \quad (3.11)$$

We consider now a path where the hopping transitions do not occur explicitly and the scattering processes take place at τ_i and n_i $(i=1,\ldots,N_s)$. Furthermore we must assume that the particle starts and finishes at the same place $n_0=n_{N_v+1}$ at time $\tau_0=0$ and $\tau_{N_v+1}=\beta$, respectively. We apply the formula (3.11) for the time intervals $(0,\tau_1),(\tau_1,\tau_2),\ldots,(\tau_{N_v},\beta)$ with variables $\theta_0,\theta_1,\ldots,\theta_{N_v}$ and formally we define $\theta_{N_v+1}=\theta_0$.

The contribution of that path to the partition function is

$$Z_{N_v}=(-1)^{N_v}v^{N_v}\sum_{\{\mu\},\{s\}}R\int_0^\beta d\tau_{N_v}\cdots\int_0^{\tau_{i+1}-\tau_0}d\tau_i\cdots\int_0^{\tau_2-\tau_0}d\tau_1\tau_0^{-N_v}\int_{-\pi}^{\pi}\frac{d\theta_{N_v}}{2\pi}\cdots\int_{-\pi}^{\pi}\frac{d\theta_0}{2\pi} \times\exp\left[i\sum_{i=1}^{N_v+1}n_i[(\theta_{i-1}-\theta_i)-2Q\mu_i]+2y\sum_{i=0}^{N_v}\cos\theta_i\frac{\tau_{i+1}-\tau_i}{\tau_0}+\sum_{s,\mu}\sum_{\substack{i,j\\(i<j)}}T^i_{s\mu}T^j_{s\mu}\ln\frac{\tau_j-\tau_i}{\tau_0}\right]\ , \quad (3.12)$$

where following Yuval and Anderson,[23] we modified the upper limits of the integrals in Eq. (3.6) by introducing the cutoff time τ_0 in order to avoid interaction points closer than τ_0. In this way the application of the form of the electron Green's function given by Eq. (2.11) in Eq. (3.2) is justified. See the discussion Sec. V for further detail.

The advantage of using the variables θ is obvious. The expression (3.11) plays the role of the particle propagator, where θ is the dimensionless momentum of the particle and $\varepsilon=-2y\cos\theta$ is the tight-binding band energy. Thus the presented hopping formalism reflects the correct band motion. Furthermore, in Eq. (3.12), θ_i is the dimensionless momentum of the particle in the time interval (τ_{i+1},τ_i).

The form of Z_{N_v} given by Eq. (3.12) still depends on the positions n_i of the particle at electron scattering processes occurring at time τ_i. Thus the summation with respect to n_i must be carried out on an infinite chain. That leads to a Dirac function $\sum_{r=0,\pm1,\pm2,\ldots}\delta(\theta_{i-1}-\theta_i+2Q\mu_i+2\pi r)$, where $2Q\mu_i$ is the momentum gained by the electron scattered at times τ_i. That Dirac δ function expresses the conservation of the momenta at the scattering process with ambiguity of a reciprocal lattice vector $2\pi r$. Now we perform the integrals with respect to θ_i except the one for θ_0. The integer numbers r do not occur in the expression obtained by us as θ_i occurs only in the expressions of the band energy. In the final form we have to take the summation over the number N_v of the scattering processes and we get the following expression for the partition function Z given by Eq. (2.5)

$$Z=\sum_{N_v=0}^{\infty}(-1)^{N_v}\left[\frac{v}{\tau_0}\right]^{N_v}\sum_{\{\mu\},\{s\}}R\int_{-\pi}^{\pi}\frac{d\theta_0}{2\pi}\int_0^\beta d\tau_N\cdots\int_0^{\tau_{i+1}-\tau_0}d\tau_i\cdots\int_0^{\tau_2-\tau_0}d\tau_1\exp\left[2y\sum_{i=0}^{N_v}\cos\theta_i\frac{\tau_{i+1}-\tau_i}{\tau_0} +\sum_{\substack{i,j\\(i<j)}}\sum_{s,\mu}T^i_{s\mu}T^j_{s\mu}\ln\frac{\tau_j-\tau_i}{\tau_0}\right]\ , \quad (3.13)$$

where

$$\theta_i=\theta_{i-1}-2Q\mu_i \ , \tag{3.14}$$

thus

$$\theta_i=\theta_0-2Q\sum_{j=1}^{i}\mu_i \quad (i=1,\ldots,N_v) \tag{3.15}$$

is the momentum of the particle in the time interval (τ_i,τ_{i-1}) disregarding the ambiguity due to the reciprocal vectors. The only integral remaining is taken with respect to the momentum θ_0 of the particle in the initial state.

Finally, we must emphasize that the momentum conservation of the particle appears in Eq. (3.14) only with a limited accuracy because the momentum change due to a backscattering is approximated by $\pm 2k_F$ ($2Q=2k_Fb$), and the deviations of the initial and final momenta from the Fermi momenta are dropped.

C. Scaling equations

The Anderson, Yuval, and Hamann[24] scaling technique is based on elimination of the short-time behavior by increasing the short-time cutoff from τ_0 to $\tau_0+d\tau_0$ and on compensating the change in the partition function given by Eqs. (3.13)–(3.15) by introducing new values of the parameters v and y in order to keep the partition function Z invariant. We will assume that $y,v\ll 1$ and we construct the scaling equations for $\ln v$ and $\ln y$ with accuracy, where we ignore the terms $O(v^2),O(vy)$ and $O(v^3),O(y^3),O(v^2y),O(vy^2)$, respectively. The effect of changing the cutoff appears in two different ways: (i) the explicit dependence on τ_0, (ii) elimination of pairs of interaction points $(i,i+1)$ for which $\tau_0<(\tau_{i+1}-\tau_i)<\tau_0+d\tau_0$ holds.

(i) The explicit dependence is compensated if the following quantities are invariant:

$$y/\tau_0=\text{invariant} \tag{3.16}$$

and

$$\left[\frac{v}{\tau_0}\right]^{N_v}\prod_{\substack{i,j\\(i<j)}}\left[\frac{\tau_j-\tau_i}{\tau_0}\right]^{\Sigma(i,j\,|\,s\mu)}=\text{invariant} \ , \tag{3.17}$$

where the latter is considered for a given configuration and $\Sigma(i,j\,|\,s\mu)=\sum_{s,\mu}T^i_{s\mu}T^j_{s\mu}$. The exponent in Eq. (3.17) can be evaluated as

$$\sum_{s,\mu}\sum_{\substack{i,j\\(i<j)}}T^i_{s\mu}T^j_{s\mu}=\sum_{s,\mu}\left[\tfrac{1}{2}\sum_i T^i_{s\mu}\sum_j T^j_{s\mu}-\tfrac{1}{2}\sum_i (T^i_{s\mu})^2\right]$$
$$=-N_s \tag{3.18}$$

since $\sum_i T^i_{s\mu}=0$, and considering a given vertex i the term $(T^i_{s\mu})^2=1$ for two pairs of (s,μ) indices; otherwise that is zero. Thus, considering Eqs. (3.17) and (3.18) the coupling v must be invariant. Thus the scaling due to the explicit dependence on τ_0 can be written as

$$\left[\frac{\partial \ln y}{\partial \ln \tau_0}\right]_{\text{expl}}=1 \tag{3.19}$$

and

$$\left[\frac{\partial \ln v}{\partial \ln \tau_0}\right]_{\text{expl}}=0 \ . \tag{3.20}$$

(ii) First we consider a close pair p',p for which $\tau_0<(\tau_{p'}-\tau_p)<\tau_0+d\tau_0$ and the total charge is zero $T^{p'}_{s\mu}+T^{p}_{s\mu}=0$ for arbitrary index pair s,μ and we will discuss pairs of other types later. We write the partition function Z'_{N_v} with not more than one close pair of the type described as a product of the partition function Z_{N_v} with N_v scattering vertex and without close pair and of a correction factor which contains the close pair contribution in any of the intervals (τ_{i+1},τ_i) with $i=0,\ldots,N_v$. Using Eq. (3.13) we get

$$Z'_{N_v}=Z_{N_v}\left\{1+\left[\frac{v}{\tau_0}\right]^2\sum_{i=0}^{N_v}\sum_{\{\mu\},\{s\}}\int_{\tau_i+\tau_0}^{\tau_{i+1}-2\tau_0}d\tau_p\int_{\tau_p+\tau_0}^{\tau_p+\tau_0+d\tau_0}d\tau_{p'}\prod_{k=1}^{N_v}\left|\frac{\tau_k-\tau_p}{\tau_0}\right|^{\Sigma(k,p\,|\,s'\mu')}\right.$$
$$\times\prod_{l=1}^{N_v}\left|\frac{\tau_l-\tau_{p'}}{\tau_0}\right|^{\Sigma(l,p'\,|\,s''\mu'')}$$
$$\left.\times\exp\left[2y\left\{-\cos\theta_i\frac{\tau_{i+1}-\tau_i}{\tau_0}+\cos\theta_i\frac{\tau_p-\tau_i}{\tau_0}\right.\right.\right.$$
$$\left.\left.\left.+\cos\theta_p\frac{\tau_{p'}-\tau_p}{\tau_0}+\cos\theta_{p'}\frac{\tau_{i+1}-\tau_{p'}}{\tau_0}\right\}\right]\right\} , \tag{3.21}$$

where the combination factor R does not enter for the pair with zero charge as the associated Fermi operators have the structure $a^\dagger_{s\mu}a_{s\bar{\mu}}a^\dagger_{s\bar{\mu}}a_{s\mu}$; furthermore θ_i, θ_p, and θ_p are the dimensionless momenta in the intervals (τ_i,τ_p), $(\tau_p,\tau_{p'})$, and $(\tau_{p'},\tau_{i+1})$, respectively. We have to sum over all the possible $\{s\}$ and $\{\mu\}$ configurations of the pair. The first $\cos\theta_i$ term with the minus sign in Eq. (3.21) just compensates the similar unnecessary factor in Z'_{N_v}. We can expand the factors in the product appearing in Eq. (3.21) for small τ_0 and we obtain

$$\left[\frac{\tau_k-\tau_p}{\tau_0}\right]^{\Sigma(k,p\,|\,s'\mu')}\left[\frac{\tau_k-(\tau_p+\tau_0)}{\tau_0}\right]^{-\Sigma(k,p\,|\,s''\mu'')}=\left[1+\frac{\tau_0}{\tau_k-\tau_p}\sum_{s',\mu'}T^k_{s'\mu'}T^p_{s'\mu'}\right], \tag{3.22}$$

where $T^{p'}_{s\mu}=-T^p_{s\mu}$ and $|\tau_i-\tau_p|\gg\tau_0$ as a consequence of $v\ll 1$ is assumed. Furthermore, taking into account Eq. (3.15), the possible $\{\mu\}_{\text{pair}}$ configuration corresponds to $\theta_p=\theta_i\pm 2Q$ and $\theta_{p'}=\theta_p\mp 2Q=\theta_i$. Therefore, the exponential term in Eq. (3.21) can be rewritten and expanded for $y\ll 1$ as

$$\exp\{2y[\cos(\theta_i\pm 2Q)-\cos\theta_i]\}\sim\{1+2y[\cos(\theta_i\pm 2Q)-\cos\theta_i]\}\ . \tag{3.23}$$

A typical distance between interaction points is larger than $\tau_0 v^{-1}$, e.g., $|\tau_k-\tau_p|\gtrsim\tau_0 v^{-1}$, therefore the correction term on the right-hand side of Eq. (3.22) is of the order of $v\ll 1$. The partition function Z'_{N_v} given by Eq. (3.21) can be expanded simultaneously in parameters v and y by using Eqs. (3.22) and (3.23); then we get

$$Z'_{N_v}=Z_{N_v}\left[1+d\tau_0\left[\frac{v}{\tau_0}\right]^2\sum_{\{\mu\}_{\text{pair}}}\sum_{\{s\}_{\text{pair}}}\sum_{i=0}^{N_v}\int_{\tau_i+\tau_0}^{\tau_{i+1}-2\tau_0}d\tau_p\left[1+\sum_{k=1}^{N_v}\frac{\tau_0}{\tau_k-\tau_p}\sum_{s',\mu'}T^k_{s'\mu'}T^p_{s'\mu'}+2y[\cos(\theta_i-2Q\mu_p)-\cos\theta_i]\right.\right.$$
$$\left.\left.+O(v^4)+O(v^3y)+O(v^2y^2)\right]\right]. \tag{3.24}$$

Now we can perform the summation over the configuration $\{s\}_{\text{pair}}\{\mu\}_{\text{pair}}$, which gives zero for the charge $T^p_{s'\mu'}$. Using Eq. (3.14) we get

$$Z'_{N_v}=Z_{N_v}\left[1+d\tau_0\left[\frac{v}{\tau_0}\right]^2 N_s\left[2\beta+2y\sum_{i=0}^{N_v}(\tau_{i+1}-\tau_i)[\cos(\theta_i+2Q)+\cos(\theta_i-2Q)-2\cos\theta_i]\right]\right], \tag{3.25}$$

where we assumed that $\tau_{i+1}-\tau_i\gg\tau_0$, and N_s denotes the spin degeneracy of the electrons ($N_s=2$). The factor independent of τ_i provides a simple renormalization of the amplitude of Z'_{N_v}. The only relevant factor is proportional to $\cos\theta_i$, and that can be embodied into the fugacity y in (3.13) as

$$\left[\frac{d\ln y}{d\ln\tau_0}\right]_{\text{pair}}=2N_s v^2(\cos 2Q-1)=-4N_s v^2\sin^2 Q\ , \tag{3.26}$$

and obviously

$$\left[\frac{\partial\ln v}{\partial\ln\tau_0}\right]_{\text{pair}}=0 \tag{3.27}$$

holds.

Thus the final scaling equations are obtained by combining Eqs. (3.19), (3.20), (3.26), and (3.27), and they have the final form

$$\frac{\partial v}{\partial\ln\tau_0}=0+O(v^3)+O(v^2y) \tag{3.28}$$

and

$$\frac{\partial\ln y}{\partial\ln\tau_0}=1-4N_s v^2\sin^2 Q+O(v^3)+O(v^2y)\ . \tag{3.29}$$

Finally, we have to comment on the elimination of pairs with nonvanishing total charge. The elimination of those pairs is associated with generation of two-electron interaction with electron indices (s,μ) all different. In the Lee equations of these new vertices the generators are proportional to v^2, and it can be shown[26] that the generated new vertices have an upper bound proportional to v^2. The generated two-electron interaction may appear on the second power in the right-hand sides of Eqs. (3.28) and (3.29), but that is negligible. In that way vertexes of higher orders are generated as well. The physical meaning of the $\sin^2 Q$ term in Eq. (3.29) will be discussed in Sec. V.

The diagrammatic meanings of the eliminated pairs are demonstrated in Fig. 2. If the total charge is zero then the lines entering and leaving the pair have the same indices, they may play the role of a correction of self-energy type in agreement with Eq. (3.29).

IV. PARTITION FUNCTION AND SCALING IN ARBITRARY DIMENSION

The method presented in Sec. III can be generalized to arbitrary dimension. We will use the general form of the Green's function given by (2.11) where the direction of the momentum of the electron given by the unit vector $\hat{\kappa}$ and that replaces the indices $\mu=\pm 1$ used in Sec. III.

Formally the expectation value of the electron creation and annihilation operators in the expression of the partition function can be given in terms of Cauchy determinants, where the determinants are formed by Green's function with the same indices $s,\hat{\kappa}$. In dimension, $d>1$, however, electron lines with the same direction $\hat{\kappa}$ can not occur more than once in the limit of infinite volume $L\to\infty$, thus the use of a determinant is unnecessary. The charge $T_{s\hat{\kappa}}$ is defined in an analogous way to Eq. (3.4). The configuration $\{\mu\}$ is replaced by $\{\hat{\kappa},\hat{\kappa}'\}$ where the ingoing direction $\hat{\kappa}_i$ can be associated with an arbitrary outgoing $\hat{\kappa}'_i$ in contrast to the 1D case, where the ingoing direction determines the outgoing one for backscattering. In general the dimensionless coupling $v_{\hat{\kappa}\hat{\kappa}'}$ depends also on both the ingoing and outgoing

directions $\hat{\kappa}$ and $\hat{\kappa}'$. In the procedure of summing up the different hopping paths the identity (3.10) must be applied for all directions separately, and θ_i^ν means the corresponding component of the dimensionless momentum with $\nu=1,2,\ldots,d$, where d stands for the dimension. The sites of the interaction are denoted by $\mathbf{n}(\tau_i)$, which has d component and each is an integer. The expressions analogous to Eqs. (3.13) and (3.15) are

$$Z=\sum_{N_v=1}^{\infty}(-1)^{N_v}L^{-(d-1)N_v}\sum_{\{\hat{\kappa},\hat{\kappa}'\}}\sum_{\{s\}}R\int_{-\pi}^{\pi}\frac{d\theta^1}{2\pi}\cdots\int_{-\pi}^{\pi}\frac{d\theta^\nu}{2\pi}\int_0^\beta d\tau_N\cdots\int_0^{\tau_{i+1}-\tau_0}d\tau_i\cdots\int_0^{\tau_2-\tau_0}d\tau_1$$
$$\times\exp\left[2y\sum_{i=0}^{N_v}\left[\sum_{\nu=1}^{d}\cos\theta_i^\nu\right]\frac{\tau_{i+1}-\tau_i}{\tau_0}+\sum_{\substack{i,j\\(i<j)}}\sum_{s,\hat{\kappa}}T^i_{s\hat{\kappa}}T^j_{s\hat{\kappa}}\ln\frac{\tau_j-\tau_i}{\tau_0}\right], \tag{4.1}$$

where

$$\theta_i^\nu=\theta_{i-1}^\nu-Q(\kappa_i^\nu-\kappa_i'^\nu)\quad(\nu=1,\ldots,d)\,. \tag{4.2}$$

In deriving the scaling equations, special attention must be paid only to the elimination of pairs. The contribution of a close pair with zero charge can be given by a form similar to Eq. (3.24) as

$$Z'_{N_v}=Z_{N_v}\left[1+\frac{d\tau_0}{\tau_0}\sum_{\{s\}_{\text{pair}}}\sum_{\{\hat{\kappa},\hat{\kappa}'\}_{\text{pair}}}|v_{\hat{\kappa}_p\hat{\kappa}'_p}|^2\sum_{i=0}^{N_v}\int_{\tau_i-\tau_0}^{\tau_{i+1}-2\tau_0}d\tau_p\left[1+\sum_{k=1}^{N_v}\frac{\tau_0}{\tau_k-\tau_p}\sum_{s'',\hat{\kappa}''}T^k_{s''\hat{\kappa}''}T^p_{s''\hat{\kappa}''}\right.\right.$$
$$\left.\left.+2y\sum_{\nu=1}^{d}\{\cos[\theta_i^\nu-Q(\hat{\kappa}_p^\nu-\hat{\kappa}_p'^\nu)]-\cos\theta_i^\nu\}\right]\right], \tag{4.3}$$

where $v_{\hat{\kappa}_p\hat{\kappa}'_p}=\rho V_{\hat{\kappa}_p\hat{\kappa}'_p}$ and $V_{\hat{\kappa}_p\hat{\kappa}'_p}$ is the interaction matrix element between directions $\hat{\kappa}'_p$ and $\hat{\kappa}_p$ at time τ_p. This expression can be written in a more simple form if the expression following the integral symbol is symmetrized in the configuration space in the sense that the incoming and outgoing directions $\hat{\kappa}'_p$ and $\hat{\kappa}_p$ are interchanged at both scattering points of the pair. The term in the middle proportional to $T^p_{s''\hat{\kappa}''}$ is canceled by symmetrization, and the last one becomes proportional to $\cos\theta_i^\nu$. Thus we have correction due to a close pair with zero change

$$Z'_{N_v}=Z_{N_v}\left\{1+\frac{d\tau_0}{\tau_0}\sum_{\{s\}_{\text{pair}}}\sum_{\{\hat{\kappa},\hat{\kappa}'\}_{\text{pair}}}\left|v_{\hat{\kappa}'_p\hat{\kappa}_p}\right|^2\left[\beta-4y\sum_{i=0}^{N_v}\frac{\tau_{i+1}-\tau_i}{\tau_0}\sum_{\nu=1}^{d}\cos\theta_i^\nu\sin^2\left[\frac{Q}{2}(\hat{\kappa}^\nu-\hat{\kappa}'^\nu)\right]\right]\right\}. \tag{4.4}$$

Thus, the elimination of a close pair with zero total charge can be compensated by changing y in expression (4.1)

$$\left[\frac{d\ln y}{d\ln\tau_0}\right]_{\text{pair}}=-2N_sL^{-2(d-1)}\sum_{\hat{\kappa},\hat{\kappa}'}|v_{\hat{\kappa},\hat{\kappa}'}|^2\sin^2\left[\frac{Q}{2}(\hat{\kappa}^\nu-\hat{\kappa}'^\nu)\right], \tag{4.5}$$

where ν stands for an arbitrary direction in the isotropic case.

Our previous result for $d=1$ given by Eq. (3.25) is a special case of the expression above.

Turning to the close pairs with nonvanishing total charge, two cases must be distinguished. In the first case the pair involves four electrons with different indices $(s,\hat{\kappa})$ and in the second case the same index belongs to a creation and an annihilation operator and the other two indices are different. In the first case electron-electron interaction is generated, which does not contribute to the scaling equations for y and $v_{\hat{\kappa}\hat{\kappa}'}$ in our approximation schema as that has been discussed in Sec. III. The second case appears only for $d>1$, as in dimension $d=1$ there are only two different orbital indices for a given spin. In the second case the interaction $v_{\hat{\kappa}\hat{\kappa}'}$ may be generated, thus that may contribute to the scaling equation for $v_{\hat{\kappa}\hat{\kappa}'}$.

The interaction $v_{\hat{\kappa}\hat{\kappa}'}$ is generated by two different pairs which can be characterized by their interaction at times τ_{p+1} and τ_p as $v_{\hat{\kappa}\hat{\kappa}''}v_{\hat{\kappa}''\hat{\kappa}'}$ and $v_{\hat{\kappa}''\hat{\kappa}'}v_{\hat{\kappa}\hat{\kappa}''}$. Those two pair contributions due to the direction $\hat{\kappa}''$ to the interaction of that pair with another interaction point of the $\tau_{\hat{k}}$ cancel each other with logarithmic accuracy because the combinational factor $R=\pm1$ has different values for those two pairs. The remaining interaction is due to directions $\hat{\kappa}$ and $\hat{\kappa}'$ that has just the form which is characteristic for a vertex $v_{\hat{\kappa}\hat{\kappa}'}$ (see Fig. 2).

Now we consider the close pair with times τ_{p+1} and τ_p in the time interval (τ_i,τ_{i+1}). By the eliminations of that pair the band-energy terms proportional to $y\cos\theta_i^\nu$ may be changed in Eq. (4.1). That possible change arises from the time interval (τ_p,τ_{p+1}) which has the length τ_0. The dimensionless momenta of the particle in those intervals

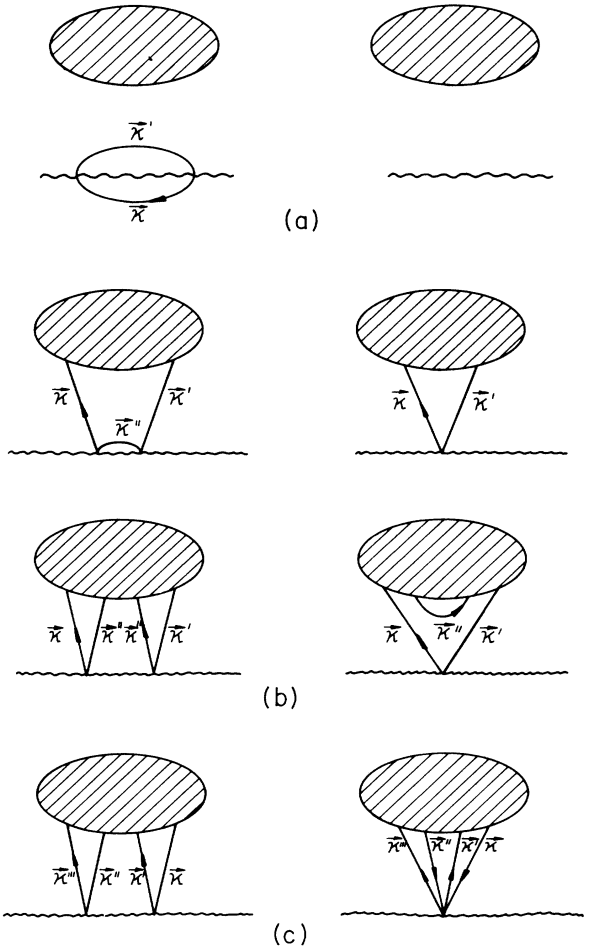

FIG. 2. Different diagrams are depicted which illustrate the elimination of the short-time behavior: first a diagram with and second the diagram without the short-time insertion. The wavy line represents the particle, which also indicates the time flow. The shadowed area represents the electronic part of the diagram which is connected with the particle line several times, but here only the different short-time insertion is shown which can be eliminated and compensated for by different renormalizations: (a) typical self-energy diagram which provides the main contribution to the renormalization of the particle; (b) the two interaction points of short-time difference can be replaced by a renormalized vertex. The renormalized diagrams can be different depending on whether the line with momentum κ'' connects directly the two interaction points or is connected also with the remaining electronic part. In the latter case the two disconnected lines with momentum κ'' must be closed. (c) If all of the momenta κ, κ', κ'', and κ''' are different then a new vertex with four electronic legs must be introduced, but the latter cases do not play an important role in the present schema.

are $\theta_i^\nu+Q(\hat{\kappa}_p^\nu-\hat{\kappa}_p'^\nu)$ and $\theta_i^\nu+Q(\hat{\kappa}_p''^\nu-\hat{\kappa}_p'^\nu)$ for the two different pairs, respectively.

The contribution of the second pair has an additional negative sign due to the different order of the operators $a_{s\hat{\kappa}'}^\dagger$ and $a_{s\hat{\kappa}}$ (see the definition of the combinational factor R in part A of Sec. III). The momenta to be associated with that time point in that interval is ambiguous after the elimination of the pair, as those depend where the generated new interaction is placed in the interval (τ_{p+1},τ_p). However, by expanding the strength of the generation of the interaction $v_{\hat{\kappa}\hat{\kappa}'}$ with respect to $y\ll 1$ we get a contribution which is proportional to $yv_{\hat{\kappa}\hat{\kappa}''}v_{\hat{\kappa}''\hat{\kappa}'}$ which is of the order of $O(v^2y)$. The correction of that order is beyond our approximation [see Eq. (3.8)], thus the ambiguity does not lead to any further complication.

Thus, in dimensions $d>1$ like in case $d=1$ only the fugacity y is renormalized, and by combining the explicit and pair contributions the final result is

$$\frac{d\ln y}{d\ln\tau_0}=1-2N_sL^{-2(d-1)}\times\sum_{\hat{\kappa},\hat{\kappa}'}|v_{\hat{\kappa}\hat{\kappa}'}|^2\sin^2\left[\frac{Q}{2}(\hat{\kappa}^\nu-\hat{\kappa}'^\nu)\right]. \quad (4.6)$$

The consequences of the scaling equations obtained will be discussed in Sec. V.

V. RESULTS AND DISCUSSIONS

In this section we give a detailed discussion of the results obtained.

The method presented here is restricted to zero temperature as the electron Green's function given by Eq. (2.11) does not depend on temperature. The length of the imaginary time axis $\beta=(kT)^{-1}$ appears only for formal convenience.

A. Cutoff

The short-time cutoff τ_0 occurs in two different ways in our formalism: (i) the electron bandwidth cutoff $\tau_D^{-1}=D$, (ii) the finite instanton width $\tau_{\rm ins}$ for the tunneling from one site to the next neighboring site in the complex time path integral method.

We have to take the larger of these two quantities $\tau_0=\max\{\tau_D,\tau_{\rm ins}\}$. The instanton width can be estimated by considering a tunneling process through a squarelike barrier with width $d_{\rm bar}$ and potential height $V_{\rm bar}$ as $\tau_{\rm ins}\sim d_{\rm bar}(2V_{\rm bar}/m)^{-1/2}$ where m is the mass of the hopping particle. The quantity $\tau_{\rm ins}$ can be of the order of the Fermi energy for an electron, as the bare electron mass must be substituted. For muons or hydrogen, however, $\tau_0\sim\tau_{\rm ins}\gg\tau_D=D^{-1}\sim\varepsilon_F^{-1}$ as the mass m is much larger, thus $\tau_{\rm ins}$ can be larger than τ_D at least by one order of magnitude.

The cutoff τ_0 occurred in two different places in our formalism: (i) the condition for validity of the Green's function given by Eq. (2.11), (ii) in the expression (3.12) for the partition function as the cutoff in the upper boundaries of the integrals.

In the first case we have to find the necessary condi-

tion for $|R-R'| \ll |\tau-\tau'| v_F$. The shortest possible time to make a distance equivalent to $|R-R'|/b$ sites is $|\tau-\tau'| > \tau_0(R-R')/b$, thus the condition is $\tau_0 v_F/b \gg 1$, which is approximately equivalent $\tau_0 \varepsilon_F \gg 1$. Thus the approximate form of the Green's function (2.11) holds for almost the entire time scale. Considering the second case, τ_0 plays the role of the shortest time between scattering processes. That time is not necessarily $\tau_{\rm ins}$, as we have placed several tunneling events between the scatterings. The order of magnitude of τ_0 is correct again except the case where there are very many tunnelings between two scatterings ($y \gg v$) with the average value y/v, and in that case $\tau_0 = \tau_{\rm ins} y/v$ must be taken.

For large degeneracy $N_s \gg 1$, the validity of the present theory is given by $y \ll 1$ and $v/N_s \ll 1$. The latter modification is justified, as the average time between scatterings with the same color is $N_s v^{-1} \tau_0$, which appears in the condition for using the long-time approximation for the Green's functions.[30]

B. Scaling equations

The scaling equations for the coupling v and the hopping fugacity have been derived with accuracy $O(v^3)$ and $O(v^2 y)$, where the approximation for v corresponds to the leading logarithmic one and that for y holds in the next-to-the-leading one, and where y is the first nonvanishing one. In general to get the self-energy y with that accuracy the vertex v must be calculated in the leading order.

The results obtained and given by Eqs. (3.28), (3.29), and (4.6) can be summarized for arbitrary dimension $d = 1,2,3$ as

$$v \equiv \text{invariant} \tag{5.1}$$

and

$$\frac{d\ln y}{d\ln \tau_0} = 1-K \ , \tag{5.2}$$

where

$$K = 4N_s v^2 \sin^2 Q \quad \text{for 1D} \ , \tag{5.2a}$$

$$K = N_s v^2 [1 - J_0^2(Q)] \quad \text{for 2D} \ , \tag{5.2b}$$

$$K = N_s v^2 [1 - j_0^2(Q)] \quad \text{for 3D} \ , \tag{5.2c}$$

$$= N_s v^2 \left[1 - \frac{\sin^2 Q}{Q^2} \right]$$

are obtained by performing the integrals in Eq. (4.6) where J_0 and j_0 are the Bessel and the spherical Bessel functions of first kind. These equations have many interesting features.

(i) The single coupling v responsible for screening is not renormalized as in many other models. The enhancement of the couplings in the order of v^2 is always due to the noncommutative nature of several different couplings like in the Kondo problem or in the case of the TLS.[7] Even in the commutative case of the TLS[31,26] there is a term on the rhs of the scaling equation proportional to vy^2. That correction does not occur in the present case similarly to the 1D hopping motion coupled to a 1D electron gas with only forward electron scattering as that has been discussed by Itai.[21] He has shown that the contributions of any hopping step and of the step in the opposite direction cancel each other, which cannot happen in the two-site problem (TLS). That difference appears as a formal consequence in the methods applied for these two cases; namely, hopping pairs are not eliminated in the method presented here, thus all corrections are proportional at least to v^2 and, therefore, corrections proportional vy^2 cannot exist.

(ii) The bandwidth of the hopping particle $\Delta = y/\tau_0$ always decreases due to the scaling ($K > 0$). Considering Eq. (5.2), two cases are distinguished: $K < 1$ where y increases, and $K > 1$ where y decreases. Our theory for $N_s = 2$ is adequate only in the case $K < 1$, but the discussion of the case $K > 1$ is also instructive, as will be discussed later. These cases are also known at zero temperature as the case of nonlocalization (band motion) and of localization, respectively. In the first case the scaling can be applied until $y = 1$ is reached, when the inverse time cutoff τ_0^{-1} starts to exceed the renormalized hopping rate Δ. That condition can be obviously interpreted for the two-site problem; in the general case, however, we can simply argue formally that our theory is valid only if $y \ll 1$. Considering the boundary of the scaling region, the self-consistent solution of Eq. (1.2) for the critical value Δ_c has been obtained by several authors and the result is

$$\Delta_c = \Delta_0 \left[\frac{\Delta_0}{D} \right]^{K/(1-K)} \ . \tag{5.3}$$

In the second case $K < 1$ the y scales to zero, thus the hopping is absent in the scaled partition function at $T = 0$. The extrapolation for large K can be justified especially in the limit $N_s \gg 1$.

(iii) In the case of the Kondo problem or of the TLS with electron assisted tunneling,[7] the strength of logarithmic interaction between scattering processes depends on the phase shift, which is therefore strongly renormalized. In the present case such renormalization does not occur, as that strength depends on the charges T in expression (3.14) or (4.1) where T has kinematical origin only.

C. Comparison with the two-site model and extrapolation for $K > 1$

Considering the many-site problem there is a widely expected conjecture,[1,17] that to determine the bandwidth y is enough to calculate the renormalized hopping rate in the two-site problem. Concerning the hopping rate y the final results given by Eqs. (5.2) and (5.2a)–(5.2c) coincide with the scaling equations of the two-site problem with screening only, thus without assisted tunneling. The geometrical factor in the interaction matrix element $\frac{1}{2}(e^{i(\mathbf{k}-\mathbf{k}')\cdot\mathbf{a}_1} - e^{i(\mathbf{k}-\mathbf{k}')\cdot\mathbf{a}_2})$ must be taken into account, however, for an arbitrarily large separation distance between the two sites. Here $\mathbf{k}-\mathbf{k}'$ is the momentum transfer; furthermore, $\mathbf{a}_1$ and $\mathbf{a}_2$ stand for the positions of the two sites.[7] We have learned by studying the two-site problem that for $d > 1$ Eqs. (5.2b) and (5.2c) can be applied for ar-

bitrarily strong coupling in a single angular momentum channel, e.g., $l=0$ if the coupling is replaced by δ_l/π where δ_l is the phase shift defined as $\delta=-\arctan(\pi v)$. That result very strongly supports the extrapolation of the scaling Eq. (5.2) for $K>1$ with an appropriate definition of K for strong coupling $K\gtrsim 1$.

D. Role of Friedel oscillation

Comparison of the 1D models with only forward scattering or with only backscattering in the absence of infrared corrections in the scaling equation in the first case strongly suggests that the infrared term given by Eq. (5.2a) is due to the formation of the Friedel oscillation in the density of the electrons which is proportional to $\sin(2k_F r)/r$ where r is the distance measured from the particle. The periodicity of that oscillation is $2\pi(2k_f)^{-1}$. From Eq. (5.2a) it is evident that if the hopping distance is $b=2\pi(2k_F)^{-1}n$, where $n=0,\pm1,\pm2,\ldots$, then $K=0$.[32] In other words, if the Friedel oscillations are in phase before and after hopping, then only their amplitude is modified and that is negligible in large distance. For any other value of b, however, the whole electron screening must be rearranged. The situation is depicted in Fig. 3.

As can be seen from Fig. 4, this argument cannot be applied for cases $d>1$ as the condition of the phase coherence is different in different directions.

E. Relationship with Schmid's model

Schmid[18] has proposed a model for 1D hopping coupled to a 1D acoustic-phonon gas. The interaction Hamiltonian can be written as[19]

$$H_1=g\sum_n nc_n^\dagger c_n\sum_k k^{1/2}(b_k+b_k^\dagger)\ , \tag{5.4}$$

where g is the coupling and b_k is the Bose operator of the phonons. That Hamiltonian can be derived from Eq. (2.4) in an extreme limit assuming that the lattice constant b at the hopping lattice is very small, $bk_F\ll 1$ ($R_n=bn$), and in the localization region the position of the particle can be described by a few values of n. In that limit the exponent in Eq. (2.4) can be expanded and we keep only the term proportional to $R_n=nb$. By introducing new electron operators $A_\pm(k)=(1/\sqrt{2})(a_k+a_{-k})$ with $k>0$ the model can be transformed to a forward scattering model with two colors $\pm$ additional to the spin. That Hamiltonian can be bosonized and we get the Hamiltonian (5.4).

That equivalence holds only in a very extreme limit; the two Hamiltonians, however, belong to the same universality class with Ohmic character.[18–20]

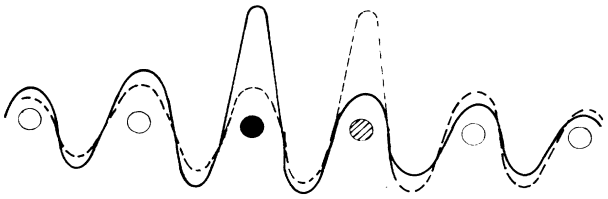

FIG. 3. The Friedel oscillations are formed around the heavy particle in positions of the solid and shadowed circles and they are represented by solid and dashed lines, respectively. If the periodicity of the Friedel oscillation coincides with the lattice constant then the Friedel oscillation with solid and dashed lines are not distinguishable at large distances in the one-dimensional model. Therefore, the renormalization given by Eq. (5.2a) disappears on the right-hand side of Eq. (5.2).

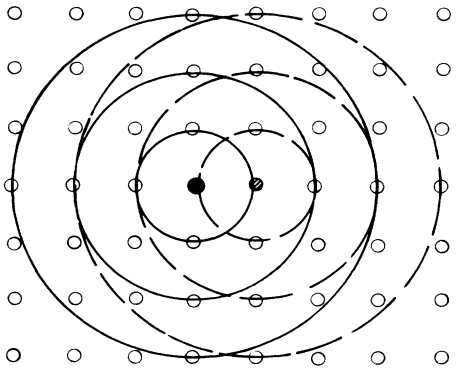

FIG. 4. The Friedel oscillations are shown for two positions of the particle by solid and dashed lines in two dimensions. At large distances the Friedel oscillations are always distinguishable, thus the strength of the renormalization given by Eq. (5.2b) cannot vanish.

F. Diffusion constant

The present theory describes the renormalized propagating motion of the particle and we get the temperature dependence of the bandwidth from the scaling equation. The partition function evaluated for $T=0$ does not include, however, the temperature-dependent damping of the particle, which is due to creations of electron-hole fermion pairs. We can get the diffusion constant by solving the classical kinetic equation with the scaled overlap integral and the invariant particle-fermion coupling. Such a kinetic equation is derived and solved by Yamada,[11] and that solution justifies the proposed combination of the path integral method with the classical kinetic equation. We emphasize that the collision term[33] and the overlap integral can be given by the same expression K of the coupling.

For further details see Ref. 16.

VI. SUMMARY

We have studied a particle moving in a periodic lattice coupled to a degenerate electron gas with large momentum transfer. In analogy with the path integral technique developed for the two-site problem we generalized that method for the periodic case. In the long-time approximation we determined the partition function of the system. By means of different summation and scaling techniques we identified two phases in the problem: for weak

coupling $K < 1$, the particle propagates with a renormalized hopping integral but the particle-electron coupling is invariant; for sufficiently large coupling $K > 1$, the extrapolated results show that the electrons freeze the particle into its initial state at temperature $T = 0$. We propose that the path-integral technique for $T = 0$ can be combined with the classical kinetic equations to get transport coefficients like the diffusion constant. We suggest that such a combined technique can be applied for some problems of the heavy fermionic systems.

We have shown that, disregarding some extreme limits, the studied Hamiltonian is different from the bosonic Hamiltonian proposed by Caldeira and Leggett to describe the coupling of the particle to a heat bath, but both problems belong to the same universality class called Ohmic dissipation.

We note that concerning some recent considerations dealing with measurement theory, the model studied here can serve as a measurement apparatus for the position of the particle in the sense suggested in Ref. 34. By switching the coupling with a large enough value $K > 1$, the particle becomes localized and its position can be measured by noninvasive measurement.

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