Direct construction of path integrals in the lattice-space multiband dynamics of electrons in a solid

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It is suggested that complex problems in ultrasubmicrometer electronics research may greatly benefit from use of the path-integral technique. The use of the Weyl-Wigner formalism of the quantum dynamics of electrons in solids provides a rigorous and straightforward derivation of the path integral in solid-state physics, both from the single-particle and from the many-body field-theoretical description of electron dynamics, without the need to postulate *a priori* the isomorphism between quantum operators and c-numbers of the base field. A rigorous construction of the path integral in many-body solid-state band theory necessitates a two-stage Weyl correspondence between quantum operators and c-numbers of the base field, namely, the Weyl correspondence of the base field of "lattice-space" particle-dynamical variables and that of the continuum many-body field-dynamical variables.

I. INTRODUCTION

A couple of observations on recent technical developments, as they potentially relate to ultrasubmicrometer electronics research (USER), has led us to examine the construction of path integrals in the lattice-space multiband dynamics of electrons in a solid: (a) The use of supercomputers for evaluating fermionic and coupled boson-fermion path integrals, for complex quantum many-body system and lattice gauge theories, has recently emerged as an exciting research activity in the last four years,[1,2] and numerical technique for carrying these calculations are gradually being established; (b) aside from its well-known classical-dynamical property, there is a problem-solving property associated with the process of defining a significant path in state space or configuration space, in the path-integral evaluation by means of computer (Monte Carlo) Metropolis importance-sampling algorithm.[3] The author believed this conceptual property to have much wider applications to problem solving in general, and in particular to artificial-intelligence (AI) research, operation research, and in discrete combinatorial optimization (i.e., NP-complete[3] complex combinatorial problems) in science and engineering.

USER is faced with essentially two seemingly insurmountable difficulties: (a) giving an accurate description of device physics in ultrasubmicrometer dimensions[4] where discreteness and/or atomicity in all physical quantities of interest dominate the device behavior; clearly in this case one needs to go beyond the continuum effective-mass dynamical theories, and (b) obtaining the solution to highly complex discrete combinatorial problems connected with the optimization of the system architectures.[5] We believe that solution to a wide range of very complex quantum dynamical and combinatorial problems in USER may be greatly benefited by both the powerful concept of the path-integral technique, together with advances in numerically evaluating it, and by the problem-solving property associated with the process of defining the most significant path in state space or configuration space.

First, let us clarify what we mean by our second observation since we will not say anything more about it in this paper beyond the first section. It is interesting to note that already highly complex (NP-complete) discrete combinatorial problems connected with the optimization of a system architecture are beginning to benefit from the problem-solving property associated with the process of defining the most significant path, in state or configuration space, in the numerical evaluation of path integrals. This has recently occurred in the literature in the guise of what Kirkpatrick, Gelatt, and Vecchi[6] have called the "annealing schedule." Table I shows the essential elements of general problem solving, and of the combinatorial optimization process in particular (third column). Elements of the fourth column, which manage to define the most significant path (calculated by means of a Monte Carlo importance-sampling technique), are shown to be isomorphic to the elements of general problem solving and of general combinatorial optimization processes. The fourth element (fourth row in the table) as stated is rather vague, but its importance cannot be underestimated. The plan is the reason for introducing search tree, search levels (i.e., depths) and nodes at each search level in a tree; in other words the fourth element is the niche for all ingenuity[7] that can be applied to the problem to efficiently coordinate the second and third element. The plan then maps out the evolution of the search toward the solution and, therefore, gives the sense of directionality. Indeed, one may view the search levels (depths) of the search tree to correspond to the "imaginary time" in statistical physics.

The isomorphism shown in Table I can indeed be seen in the work of Kirkpatrick, Gelatt, and Vecchi[6] (although they did not relate their method to a path integral) in their computer solution to some specific combinatorial problems in wire routing, macroplacement, and partitioning in computer designs, as well as to the classic traveling-

TABLE I. Elements of complexity management.

Automated problem solver in artificial intelligence (AI)		General combinatorial optimization problems	Path of minimum total action in path-integral Monte Carlo for the "ground-state configuration"
1. Given: (a) initial situation and goal	(b) Logical sentences representing premises and a theorem to be proved	1. Initial configuration (concise definition of a system; actual realization which may be far from optimum) and goal (optimum combination, minimum cost)	1. Arbitrary initial configuration and goal (ground-state configuration)
2. (a) Operators (procedures on generalized actions) that can be used for changing situations. (Random number generator may be employed here.)	(b) Symbol manipulation and rules of the logical system to be able to construct new logical statements from the old ones	2. Generation of "moves" or rearrangement of the elements in a configuration; "transformation operator" for changing configuration (random number generator may be employed here).	2. Random generator of "moves" or rearrangement of elements in the configuration (particle coordinates); random generator of "$3N$-coordinates" at each break point
3. (a) Constraints, conditions and/or heuristics to be satisfied for a specific procedure and resulting situation to be accepted, based on the characterization of each realizable situation	(b) Evaluate outcome of manipulation as either true or false; if true, accept, if false reject (fuzzy logic is an active field of research in AI)	3. Objective (cost) function evaluator containing the constraints, conditions, and/or heuristics to be satisfied for accepting the new configuration	3. Accept legal "moves" according to Boltzmann distribution function for each "break point" including the end point (Metropolis importance sampling procedures)
4. (a) Plan for synthesizing the set of actions 2(a) and 3(a) (i.e., introduce levels of search and nodes in a search tree, etc.) to serve as a "structure" in which to apply 2(a) and 3(a)	(b) Plan on strategy for carrying out 2(b) and 3(b) [i.e., construct graphs, trees and other constructs to serve as a structure for 2(b) and 3(b) to apply]	4. Plan for synthesizing set of actions 2 and 3. Levels of search correspond to "time" and nodes of search tree correspond to different configuration.	4. Select "classical path" (annealing schedule) of path-integral Monte Carlo over a very long "time" from $\tau=0$ ($T=\infty$) to $\tau\rightarrow\infty$ ($T=0$). The configuration obtained at the end point is the optimum ground-state configuration. Note: One can allow "fuzzy path" by including deviations from classical path.

salesman problem.[8] Their algorithm corresponds to the breadth-first search algorithm (a technique very well known in the study of data structures and graph algorithms and in AI research)[8] in their use of the Metropolis importance-sampling procedure for exploring the optimum configuration at each search level or "temperature." Extension of their work can be found in Ref. 9. The temperature which they have introduced, in an *ad hoc* manner, in their optimization process can be viewed as a measure of the different "levels of the search tree;" it measures the evolution (denoted in Ref. 6 the annealing schedule) toward the goal. We will not go into further discussion in this paper on the problem-solving property associated with the process of defining the most significant path in state or configuration space since clearly what remains are essentially practical and ingenious applications of this powerful and universal concept.

The main objective of this paper is to cast the quantum dynamics of electrons in a solid more accurately as a path integral from the atomistic point of view, to explicitly incorporate discreteness, and to avoid the use of continuum effective-mass dynamical theories. To the author's knowledge, this has not been explicitly treated in the literature. As we shall see in what follows, path-integral lattice-space quantum dynamics of electrons in a crystalline solid bear a very close resemblance and/or analogy with the lattice-gauge theories of elementary-particle physics. A further understanding and utilization of the existing analogy could therefore conceptually lead to a cross-fertilization of ideas, not only between quantum-field theory and statistical mechanics, but also between quantum-field theory, statistical mechanics, and USER—microstructure-science dynamical problems as well.

Path-integral solutions, in principle, can be written down for a host of evolution equations in physics.[10–14] The derivation and construction of the path integral (also known as functional integral) in quantum physics has only been of interest primarily to the people in elementary-particle physics.[15–19] The role of isomorphism between quantum operators or quantum states with the "c-numbers" of the base field is the central feature of the construction process. So far, the method is characterized by postulating the intended isomorphism (with usual assumption of normal ordering) and then giving a proof that indeed the isomorphism is one-to-one. It is not at all clear how this construction method is applicable to particles in solids, possessing multiband dynamics (more appropriately "lattice-space dynamics" owing to finite bandwidths). What is needed, and to the author's knowledge has not been done, is to eliminate the initial postulatory aspect of establishing isomorphism or Weyl correspondence between classical quantities and quantum operators in the construction of path integrals. Indeed, as we shall see, for many-body solid-state band theory the nonpostulatory Weyl correspondence is a two-stage process.

The outline of the rest of this paper is as follows. Sections II and III serve to define the first-stage Weyl correspondence via the Weyl-Wigner formalism of the quantum theory of solids, proposed by the author some years ago. Section II starts by showing that indeed in solid-state theory the most convenient basic conjugate variables are the lattice-point coordinates and crystal momentum (limited to the first Brillouin zone). For this reason, we refer to the dynamics of electrons in solids as lattice-space dynamics, a term which may acquire significant relevance for ultrasubmicron semiconductor devices. It is through the use of the Weyl-Wigner formalism which enables us to establish isomorphism between quantum operators and c-numbers of the base field, without the need to postulate *a priori* this correspondence. Section IV develops the second-stage Weyl correspondence to complete the formalism of a rigorous and straightforward approach to the construction of a path integral in solid-state physics. The method shows clearly how the construction runs parallel in both first quantization and second quantization, differences arise mainly from differences in the number of dimensions and the class of the basic conjugate dynamical variables being considered.

II. THE FIRST-STAGE WEYL CORRESPONDENCE

It was shown years ago[20,21] that an arbitrary operator $A_{\rm op}$ in solid-state band theory can be expressed in terms of the crystal momentum operator and lattice-point coordinate operators. The reader is referred to Ref. 20 and references quoted therein for the following results (we make use of Dirac ket and bra notation for the Bloch functions and Wannier functions in what follows):

$$A_{\rm op}\equiv(N\hbar^3)^{-1}\sum_{p,q,\lambda,\lambda',\sigma,\sigma'}A_{\lambda\lambda'\sigma\sigma'}(p,q)\Delta_{\lambda\lambda'\sigma\sigma'}(p,q)\ , \tag{1}$$

where $A_{\lambda\lambda'\sigma\sigma'}(p,q)$ and $\Delta_{\lambda\lambda'\sigma\sigma'}(p,q)$ are given by

$$A_{\lambda\lambda'\sigma\sigma'}(p,q)=\sum_{v}e^{(2i/\hbar)p\cdot v}\langle q-v,\lambda,\sigma\,|\,A_{\rm op}\,|\,q+v,\lambda',\sigma'\rangle\ , \tag{2}$$

$$\Delta_{\lambda\lambda'\sigma\sigma'}(p,q)=\sum_{u}e^{(2i/\hbar)q\cdot u}\,|\,p-u,\lambda,\sigma\rangle\langle p+u,\lambda',\sigma'\,|\ , \tag{3}$$

or by the equivalent expressions,

$$A_{\lambda\lambda'\sigma\sigma'}(p,q)=\sum_{u}e^{(2i/\hbar)q\cdot u}\langle p+u,\lambda,\sigma\,|\,A_{\rm op}\,|\,p-u,\lambda',\sigma'\rangle\ , \tag{4}$$

$$\Delta_{\lambda\lambda'\sigma\sigma'}(p,q)=\sum_{v}e^{(2i/\hbar)p\cdot v}\,|\,q+v,\lambda,\sigma\rangle\langle q-v,\lambda',\sigma'\,|\ . \tag{5}$$

N is the number of lattice points, p is the crystal momentum (limited to the first Brillouin zone), q is the lattice-point coordinate, σ,σ' label the spin indices, and λ,λ' label the band indices. The operator nature of $A_{\rm op}$ has been transferred to $\Delta_{\lambda\lambda'\sigma\sigma'}(p,q)$ in Eq. (1). Indeed $\Delta_{\lambda\lambda'\sigma\sigma'}(p,q)$ can be rewritten to exhibit its operator nature in terms of P and Q as

$$\Delta_{\lambda\lambda'\sigma\sigma'}(p,q)=\sum_{v,u}e^{(2i/\hbar)(q+v-Q)\cdot u}e^{(2i/\hbar)(p-P)\cdot v}\Omega_{\lambda\lambda'\sigma\sigma'}\ , \tag{6}$$

where

$$\Omega_{\lambda\lambda'\sigma\sigma'}=\sum_{q}|q,\lambda,\sigma\rangle\langle q,\lambda',\sigma'|$$
$$=\sum_{p}|p,\lambda,\sigma\rangle\langle p,\lambda',\sigma'| \ . \tag{7}$$

P and Q are the crystal momentum and lattice-point coordinate operator, respectively, they are the canonical conjugate variables suitable for solid-state problems, i.e., one can show that the following commutation relation holds:[20,21]

$$[P_l,Q_j]=\frac{\hbar}{i}\delta_{lj} \ . \tag{8}$$

The eigenvalues and eigenfunctions of Q are the lattice-point coordinates and Wannier functions, respectively. Likewise, the eigenvalues and eigenfunctions of P are the crystal momentum (limited to the first Brillouin zone) and Bloch functions, respectively. $A_{\lambda\lambda'\sigma\sigma'}(p,q)$ defined by Eq. (2) or (4) is the Weyl transform of the quantum operator $A_{\rm op}$ in the Weyl-Wigner formulation of quantum mechanics.[20,23] Referred to discrete lattice (solid-state) problems it is convenient to call $A_{\lambda\lambda'\sigma\sigma'}(p,q)$ the "lattice Weyl transform" of $A_{\rm op}$. Equations (1) and (2) can be viewed as providing us with the exact mathematical prescription for associating classical and more pictorial quantities with quantum-mechanical operators and vice versa. It should be pointed out that the corresponding classical quantities may still contain Planck's constant h. Indeed the classical-mechanical pictorialization of the classical quantities given by Eq. (2) can often be achieved only after decoupling the band of interest.[20–25]

We write down the P-Q representation of a two-body quantum operator as

$$A^{(2)}_{\rm eff}(Q,\tilde{Q},P,\tilde{P})=(N\hbar^3)^{-2}\sum_{\substack{p,q,\lambda\lambda',\sigma\sigma',u,v,\\ \tilde{p},\tilde{q},\tilde{\lambda},\tilde{\lambda}',\tilde{\sigma},\tilde{\sigma}',\tilde{u},\tilde{v}}} A^{(2)}_{[\lambda\sigma][\tilde{\lambda}\tilde{\sigma}]}(p,\tilde{p},q,\tilde{q})\exp\left[\frac{2i}{\hbar}(q+v-Q)\cdot u\right]\exp\left[\frac{2i}{\hbar}(p-P)\cdot v\right]$$
$$\times\exp\left[\frac{2i}{\hbar}(\tilde{q}+\tilde{v}-\tilde{Q})\cdot u\right]\exp\left[\frac{2i}{\hbar}(\tilde{p}-\tilde{P})\cdot\tilde{v}\right]\Omega_{[\lambda\sigma][\tilde{\lambda}\tilde{\sigma}]} \ , \tag{9}$$

where $[\lambda\sigma]$ stands for symbol strings $\lambda\sigma\lambda'\sigma'$, $[\tilde{\lambda}\tilde{\sigma}]$ for $\tilde{\lambda}\tilde{\sigma}\tilde{\lambda}'\tilde{\sigma}'$, and

$$A^{(2)}_{[\lambda\sigma][\tilde{\lambda}\tilde{\sigma}]}(p,\tilde{p},q,\tilde{q})=\sum_{v,\tilde{v}}\exp\left[\frac{2i}{\hbar}p\cdot v\right]\exp\left[\frac{2i}{\hbar}\tilde{p}\cdot\tilde{v}\right]\langle q-v,\lambda,\sigma|\,\langle\tilde{q}-\tilde{v},\tilde{\lambda},\tilde{\sigma}|\,A_{\rm op}\,|\,\tilde{q}+\tilde{v},\tilde{\lambda}',\tilde{\sigma}'\rangle\,|\,q+v,\lambda'\sigma'\rangle \ , \tag{10}$$

$$\Omega_{[\lambda\sigma][\tilde{\lambda}\tilde{\sigma}]}=\sum_{q'',\tilde{q}''}|q'',\lambda,\sigma\rangle\,|\tilde{q}'',\tilde{\lambda},\tilde{\sigma}\rangle\langle\tilde{q}'',\tilde{\lambda}',\tilde{\sigma}'|\,\langle q'',\lambda',\sigma'|\ . \tag{11}$$

Equivalent expressions corresponding to Eqs. (4) and (5) can be obtained by using the unitary lattice Fourier transformation connecting the Wannier functions to the Bloch functions.[20,21]

The formalism of the second quantization operators in solid-state band theory via the first-stage Weyl correspondence given above is discussed in Appendix A. From Eqs. (A23) and (A24), we can immediately write down the general expression for the effective Hamiltonian in q (lattice coordinate) space as

$$\mathscr{H}_{\rm eff}=\sum_{q_1,q_2,\lambda,\lambda',\sigma,\sigma'}W^{(1)}_{\lambda\lambda'\sigma\sigma'}(q_1-q_2;q_1+q_2)\psi^{\dagger}_{\lambda\sigma}(q_1)\psi_{\lambda'\sigma'}(q_2)$$
$$+\sum_{\substack{q_1,q_2,\lambda,\lambda',\sigma,\sigma',\\ \tilde{q}_1,\tilde{q}_2,\tilde{\lambda},\tilde{\lambda}',\tilde{\sigma},\tilde{\sigma}'}}W^{(2)}_{[\lambda\sigma][\tilde{\lambda}\tilde{\sigma}]}(q_1-q_2,\tilde{q}_1-\tilde{q}_2;q_1+q_2,\tilde{q}_1+\tilde{q}_2)\psi^{\dagger}_{\lambda\sigma}(q_1)\psi^{\dagger}_{\tilde{\lambda}\tilde{\sigma}}(\tilde{q}_1)\psi_{\tilde{\lambda}'\tilde{\sigma}'}(\tilde{q}_2)\psi_{\lambda'\sigma'}(q_2) \ , \tag{12}$$

where to begin with, $A^{(1)}_{\rm op}$ is the sum of electron kinetic energies, relativistic effects plus the periodic potential of the crystal lattice. $A^{(2)}_{\rm op}$ represents all the electron-electron interaction potential of the relevant electrons under consideration.

It is important to emphasize here that although the c-number quantities occurring in Eq. (12) are simply matrix elements in the Wannier-function representation of one- and two-body quantum operators, as expressed by Eqs. (A25) and (A26), respectively, there are significant calculational advantages in obtaining these c-number quantities via the first-stage Weyl correspondence, Eqs. (A21) and (A22). The Weyl-Wigner formalism of the quantum theory of solids has a built-in mechanism for the decoupling of interacting bands,[20–25] for obtaining a physically transparent Weyl transform as a power series in the electromagnetic field strength. Moreover, for very-high-field (e.g., high uniform magnetic field) quantization rules may further be applied, in the sense used by Roth[26] and Buot[27] to effectively include all powers of the magnetic field strength, to the obtained Weyl transform. Therefore, in this manner physically meaningful calculational progress can easily be made, the Wannier functions and/or Bloch functions become a little more than a formalistic tool

rather than a real calculational tool from the beginning, i.e., one does not begin by actually calculating all matrix elements between Wannier functions of the "bare" one- and two-body operators to obtain Eq. (12) above. Through the first-stage Weyl correspondence, Eqs. (A21) and (A22), one is able to start the quantum-dynamical problem from the already calculated zero-field self-consistent energy band structure.

We will restrict ourselves to normal systems, i.e., the average of products of field operators is identically zero if in the given product the number of creation operators is not equal to the number of destruction operators (e.g., ground-state Fermi-sea quantum averaging). Symmetry-breaking terms in the Hamiltonian remove the degeneracy of the statistical equilibrium state and for this case average values of field operators are no longer zero.[28] In obtaining electron-electron correlations, attention must be paid to the number of interchanges of the field operators in Eq. (12) to form combinations of nonzero averages.[29]

The idea of obtaining an optimal one-body Hamiltonian, i.e., of the form of the first term of Eq. (12), is to include all average effects of the electron-electron interaction and hence to separate out the true electron-electron correlation effects. This leads us to incorporate in the first term of Eq. (12) the following:

$$\delta\mathscr{H}_{\rm eff}^{(1)}=\sum_{\lambda,\lambda',\sigma,\sigma',q_1,q_2}\left[\sum_{\tilde\lambda,\tilde\lambda',\tilde\sigma,\tilde\sigma',\tilde q_1,\tilde q_2} W^{(2)}_{[\lambda\sigma][\tilde\lambda\tilde\sigma]}(q_1-q_2,\tilde q_1-\tilde q_2;q_1+q_2,\tilde q_1+\tilde q_2)\times\langle\psi^\dagger_{\tilde\lambda\tilde\sigma}(\tilde q_1)\psi_{\tilde\lambda'\tilde\sigma'}(\tilde q_2)\rangle\right]\psi^\dagger_{\lambda\sigma}(q_1)\psi_{\lambda'\sigma'}(q_2)$$
$$-\sum_{\lambda,\tilde\lambda',\sigma,\tilde\sigma',q_1,\tilde q_2}\left[\sum_{\tilde\lambda,\lambda',\tilde\sigma,\sigma',\tilde q_1,q_2} W^{(2)}_{[\lambda\sigma][\tilde\lambda\tilde\sigma]}(q_1-q_2,\tilde q_1-\tilde q_2;q_1+q_2,\tilde q_1+\tilde q_2)\right.$$
$$\left.\times\langle\psi^\dagger_{\tilde\lambda\tilde\sigma}(\tilde q_1)\psi_{\lambda'\sigma'}(q_2)\rangle\right]\psi^\dagger_{\lambda\sigma}(q_1)\psi_{\tilde\lambda'\tilde\sigma'}(\tilde q_2)\,, \tag{13}$$

to obtain the band-theoretic Hamiltonian. The same expression is subtracted from the second term of Eq. (12), the resulting term will then describe the true correlation between electrons. For treating correlation effects, the field-theoretical Green's function technique has proved to be a very useful tool.[30]

We will make some simplifications. Following Mattis[31] and denoting the optimal band-theoretical Hamiltonian as $\mathscr{H}_0$ and the two-body operator which describe the electron correlation by the sum of $\mathscr{H}_c$ and $\mathscr{H}_{\rm ex}$, we have

$$\mathscr{H}_{\rm eff}=\mathscr{H}_0+\mathscr{H}_c+\mathscr{H}_{\rm ex}\,, \tag{14}$$

where after a self-consistent procedure, discussed above for $\mathscr{H}_0$, we have

$$\mathscr{H}_0=\sum_{\lambda,\sigma,q_1,q_2}\tilde W^{(1)}_\lambda(q_1-q_2;q_1+q_2)\psi^\dagger_{\lambda\sigma}(q_1)\psi_{\lambda\sigma}(q_2)\,, \tag{15}$$

$$\mathscr{H}_c=\sum_{\lambda_1,\lambda_2,\sigma_1,\sigma_2,q_1,q_2} W^{(2)c}_{\lambda_1\lambda_2}(0,0;2q_1,2q_2)\hat n_{\lambda_1\sigma_1}(q_1)[\hat n_{\lambda_2\sigma_2}(q_2)-\langle n_{\lambda_2\sigma_2}(q_2)\rangle]\,, \tag{16}$$

$$\mathscr{H}_{\rm ex}=-\sum_{\substack{\lambda_1,\lambda_2,\sigma_1,\sigma_2,q_1,q_2\\ \{\lambda_1\sigma_1\}\neq\{\lambda_2\sigma_2\}}} W^{(2)\rm ex}_{\lambda_1\lambda_2}(q_1-q_2,q_2-q_1;q_1+q_2,q_1+q_2)\psi^\dagger_{\lambda_1\sigma_1}(q_1)\psi_{\lambda_1\sigma_2}(q_1)$$
$$\times[\psi^\dagger_{\lambda_2\sigma_2}(q_2)\psi_{\lambda_2\sigma_1}(q_2)-\langle n_{\lambda_2\sigma_2}(q_2)\rangle]\,. \tag{17}$$

Equation (17) can be written in a more revealing form by summing over the spin indices. The result is[31]

$$\mathscr{H}_{\rm ex}=-\sum_{\lambda_1,\lambda_2,q_1,q_2} J_{\lambda_1\lambda_2}(q_1-q_2,q_2-q_1;q_1+q_2,q_1+q_2)\{\mathbf{S}_{\lambda_1}(q_1)\cdot\mathbf{S}_{\lambda_2}(q_2)+\tfrac14 n_{\lambda_1}(q_1)[\hat n_{\lambda_2}(q_2)-\langle n_{\lambda_2}(q_2)\rangle]\}\,, \tag{18}$$

where the quantities entering in Eq. (18) are defined as

$$J_{\lambda_1\lambda_2}(q_1-q_2,q_2-q_1;q_1+q_2,q_1+q_2)$$
$$=2W^{(2)\rm ex}_{\lambda_1\lambda_2}(q_1-q_2,q_2-q_1;q_1+q_2,q_1+q_2)\,, \tag{19}$$

$$\hat n_\lambda(q)=\sum_\sigma\hat n_{\lambda\sigma}(q)\,, \tag{20}$$

$$S^z_\lambda(q)=\tfrac12[\hat n_{\lambda\uparrow}(q)-\hat n_{\lambda\downarrow}(q)]\,, \tag{21}$$

$$S^x_\lambda(q)+iS^y_\lambda(q)=\psi^\dagger_{\lambda\uparrow}(q)\psi_{\lambda\downarrow}(q)\,, \tag{22}$$

$$S^x_\lambda(q)-iS^y_\lambda(q)=\psi^\dagger_{\lambda\downarrow}(q)\psi_{\lambda\uparrow}(q)\,. \tag{23}$$

The basis states (Wannier function) used in Eqs. (15)–(17) are assumed to be the self-consistent Wannier

functions of the Hartree-Fock Hamiltonian. From Eqs. (4) and (A21), it is clear that the general dependence on crystal lattice coordinates of the matrix element in Eq. (15) reduces to dependence on the difference of lattice coordinates only. In the presence of uniform magnetic field the appropriate basis states to use are the set of magnetic Wannier functions and its associated set of magnetic Bloch functions.[20,21] It has been shown[20–23] how one can start from the self-consistent localized solution in the absence of magnetic field to the nonzero-field self-consistent localized solution, with corresponding field-dependent renormalization of the bands expressed as a power series in the magnetic field strength. Although the renormalization of the bands can only be expected to be asymptotic, it should be pointed out, however, that the existence of magnetic Wannier functions and magnetic Bloch functions can be argued on the basis of the crystal symmetry (in the presence of uniform magnetic field) alone. In general, the renormalized bands can have very complicated dependence in the magnetic field, incorporating the multiband dynamics of Bloch electrons which are very important, for example, in the theory of diamagnetism of solids.[25,32]

The form of the effective Hamiltonian in the presence of a uniform external magnetic field is formally the same as given by Eqs. (14)—(17), with additional dependence on the magnetic field strength occurring in the matrix elements. However, for $\mathscr{H}_0$ this form alone is not explicitly gauge invariant. The explicit dependence of the matrix element on the vector potential or "gauge field" is required due to the nonlocality aspect of product of field operator $\psi^\dagger(q_1)\psi(q_2)$. This observation leads us to consider the Peierls phase factor[21] of the magnetic Wannier functions.

An expression of the form

$$W(r_1,r_2)\exp\left[\frac{ie}{\hbar c}\int_{r_2}^{r_1}A(r)\cdot dr\right]\psi^\dagger(r_1)\psi(r_2)\,, \tag{24}$$

where $W(r_1,r_2)$ is a c-number, is a gauge-invariant quantity. Now if the matter fields ψ are only defined on a lattice, then Eq. (24) would read, using the mean-value theorem for the integral, as

$$W(q_1,q_2)\exp\left[\frac{ie}{\hbar c}A\left[\frac{q_1+q_2}{2}\right]\cdot(q_1-q_2)\right]\psi^\dagger(q_1)\psi(q_2)\,, \tag{25}$$

which can also be written as

$$W(q_1,q_2)\exp\left[\frac{ie}{\hbar c}A(q_2)\cdot(q_1-q_2)\right]\psi^\dagger(q_1)\psi(q_2)\,, \tag{26}$$

where the last line is obtained using Landau gauge $A(\mathbf{q})=\frac{1}{2}\mathbf{B}\times\mathbf{q}$, B is the magnetic field strength.

We apply Eq. (26) to the expression for $\mathscr{H}_0$ in Eq. (15), at the same time incorporating the dependence on the magnetic field strength B due to the field-dependent renormalization of the bands. Using the Landau gauge for the vector potential $\mathbf{A}(\mathbf{r})=\frac{1}{2}\mathbf{B}\times\mathbf{r}$, we obtain

$$\mathscr{H}_0^{(B)}=\sum_{\lambda,\sigma,q_1,q_2}\tilde{\tilde{W}}_\lambda^{(1)}(q_1-q_2;B)\exp\left[\frac{ie}{\hbar c}A(q_2)\cdot q_1\right]\times\psi_{\lambda\sigma}^\dagger(q_1)\psi_{\lambda\sigma}(q_2)\,. \tag{27}$$

The factor multiplying the field operators in Eqs. (25) and (27) is indeed the correct form of the matrix elements of a one-body Hamiltonian, with symmetry of a crystal lattice in a uniform magnetic field, between two magnetic Wannier functions[21] whose functional form is defined by

$$\omega_{\lambda\sigma}(r-q;B)=\exp\left[-\frac{ie}{\hbar c}A(r)\cdot q\right]\tilde{\omega}_{\lambda\sigma}(r-q;B)\,, \tag{28}$$

where explicit vector-potential (gauge-field) dependence is given by the well-known Peierls phase factor.[21] $\mathscr{H}_c$ and $\mathscr{H}_{\rm ex}$ do not need a gauge-field term because they are essentially "local" terms.

We may therefore write a universal effective Hamiltonian for metals, semiconductors and insulators, and magnetic and nonmagnetic crystalline solids in a uniform magnetic field as

$$\mathscr{H}_{\rm eff}=\mathscr{H}_0^{(B)}+\mathscr{H}_c^{(B)}+\mathscr{H}_{\rm ex}^{(B)}\,, \tag{29}$$

where $\mathscr{H}_0^{(B)}$ is given by Eq. (27), and $\mathscr{H}_c^{(B)}$ and $\mathscr{H}_{\rm ex}^{(B)}$ are of the same form as Eqs. (16) and (17), respectively, but with magnetic field strength dependence incorporated in the matrix elements. Equation (29) is a generalization to nonzero field of a universal $\mathscr{H}_{\rm eff}$ given by Mattis[31] in the absence of magnetic field.

III. THE EVOLUTION OPERATOR AND SUM OVER TRAJECTORIES IN BAND THEORY

This section gives the path-integral formulation of the quantum dynamics of Bloch electrons in an external electromagnetic field, from a single-particle point of view. One can define the evolution operator of the effective Schrödinger equation as

$$U(t,t_0)=\exp\left[-\frac{i}{\hbar}(t-t_0)\mathscr{H}_{\rm eff}\right]\,, \tag{30}$$

where $\mathscr{H}_{\rm eff}$ has the form of Eq. (1). As is well known,

$$|\{\exp[-(i/\hbar)(t-t_0)\mathscr{H}_{\rm eff}]\}_{mn}|^2$$

gives the probability of transition from state n at $t=t_0$ to state m at $t=t$ and provides the accurate basis of the "golden rule" for quantum transition rates.[33]

We are interested here in expressing the transition amplitude as a "lattice path integral." A well-known procedure to carry this out is to make use of the following identity obeyed by the evolution operator:

$$U(t,t_0)=\prod_{j=1}^{n+1}U(t_j,t_{j-1})\,, \tag{31}$$

where $t_{n+1}=t$. Using the completeness of the Wannier functions which we will denote by the Dirac ket and bra notation, we have

$$\langle q^* \mid U(t,t_0) \mid q_0^* \rangle = \sum_{q_1^*} \cdots \sum_{q_n^*} \prod_{j=1}^{n+1} \langle q_j^* \mid U(t_j,t_{j-1}) \mid q_{j-1}^* \rangle , \quad (32)$$

where q^* in general represents all the quantum labels of the Wannier function. By making the time intervals infinitely small or by letting $n \to \infty$, we can take advantage of the linearity, in incremental time, of the small time evolution operators to calculate the matrix elements, after which it can be written again in exponential form but this time as a c-number. In this manner, one can compose the matrix elements of a large time evolution operator from the matrix element of the small time evolution operators. We have, from Eq. (30), for infinitesimal time intervals

$$U(t_j,t_j-1) \approx 1 - \frac{i}{\hbar}(t_j - t_{j-1})\mathscr{H}_{\text{eff}} + O((t_j - t_{j-1})^2) . \quad (33)$$

To calculate this matrix element of $\mathscr{H}_{\text{eff}}$ between two Wannier functions, we need the matrix element of the Δ operator, involved in Eq. (31), as given by Eq. (5),

$$\langle q_j \lambda_j \sigma_j \mid \Delta_{\lambda\lambda'\sigma\sigma'}(p,q) \mid q_{j-1} \lambda_{j-1} \sigma_{j-1} \rangle = e^{(i/\hbar)p\cdot(q_j - q_{j-1})} \delta_{2q,q_j+q_{j-1}} \times \delta_{\lambda_j,\lambda} \delta_{\lambda'\lambda_{j-1}} \delta_{\sigma_j,\sigma} \delta_{\sigma_{j-1},\sigma'} , \quad (34)$$

so that we can write, correct to first order in $(t_j - t_{j-1})$,

$$\langle q_j \lambda_j \sigma_j \mid U(t_j,t_{j-1}) \mid q_{j-1} \lambda_{j-1} \sigma_{j-1} \rangle = (N\hbar^3)^{-1} \sum_{p,q} \exp\left[\frac{i}{\hbar} p\cdot(q_j - q_{j-1})\right] \exp\left[\frac{-i}{\hbar}(t_j - t_{j-1}) H_{(\lambda\sigma)_j(\lambda\sigma)_{j-1}}(p,q)\right] \delta_{2q,q_j+q_{j-1}} . \quad (35)$$

The matrix element of a finite time evolution operator can therefore be written as

$$\langle q^* \mid U(t,t_0) \mid q_0^* \rangle = \lim_{n\to\infty} \left[\prod_{i=1}^{n} \sum_{q_i^*}\right] \left[\prod_{i=1}^{n+1} (N\hbar^3)^{-1} \sum_{p_i}\right] \times \exp\left\{\frac{i}{\hbar} \sum_{j=1}^{n+1} (t_j - t_{j-1}) \left[p_j \cdot \frac{q_j - q_{j-1}}{t_j - t_{j-1}} - H_{(\lambda\sigma)_j(\lambda\sigma)_{j-1}}\left[p_j, \frac{q_j + q_{j-1}}{2}\right]\right]\right\} , \quad (36)$$

where $(q_j + q_{j-1})/2$ are restricted to lattice points only, as a result of carrying out the summation over q in Eq. (35). Note that in this paper the corresponding classical Hamiltonian function is rigorously obtained from the quantum Hamiltonian operator by the use of the lattice Weyl transform.

A more revealing form of Eq. (36) can be obtained if we assume an effective Hamiltonian derived from Eqs. (1)–(6) to be of the form

$$\mathscr{H}_{\text{eff}} = \frac{P^2}{2m^*} + V(Q) , \quad (37)$$

which is a Hamiltonian, for example, of a shallow impurity in a semiconductor. Then the lattice Weyl transform [Eqs. (2) or (4)] of Eq. (37) is clearly of the form

$$H_{\lambda\lambda'\sigma\sigma'}(p,q) = \frac{p^2}{2m^*} + V(q) . \quad (38)$$

Substituting Eq. (38) in Eq. (36), and completing the square in the exponent so as to make a Gaussian p summation, we are led to the well-known Feynman path integral.[13]

IV. THE SECOND-STAGE WEYL CORRESPONDENCE: PATH INTEGRAL IN MANY-BODY PROBLEMS

In order to extend the notion of sum over trajectories for the finite time evolution operator to many-body problems, whose Hamiltonians are expressed in terms of field operators as dynamical variables, we need to extend the notion of eigenfunction and eigenvalues to field operators, i.e., to canonical variables with large or infinite number of components. For Bose field operators, that is, canonical field operators which obey the usual commutation relation as P and Q do, there is no difficulty in defining the eigenfunctions and eigenvalues and the path-integral formulation is formally identical as for Hamiltonian systems expressed in terms of P and Q. For a Bose system let $\hat{\phi}(R)$ be a field operator defined on a lattice and let $\hat{\pi}(R)$ defined through the Lagrangian be a field operator which is canonically conjugate to $\hat{\phi}(R)$. Then we define eigenfunctions and eigenvalues as

$$\hat{\phi}_\lambda(R) \mid q \rangle = q_\lambda(R) \mid q \rangle , \quad (39)$$

$$\hat{\pi}_\lambda(R) \mid p \rangle = p_\lambda(R) \mid p \rangle , \quad (40)$$

where the field configuration $q_\lambda(R)$ is the eigenvalue of the field operator $\hat{\phi}_\lambda(R)$ and $p_\lambda(R)$ is the conjugate variable to $q_\lambda(R)$; λ and R label the components of $\hat{\phi}$ and $\hat{\pi}$. The vector dot product now reads

$$p\cdot q=\sum_{R,\lambda} p_\lambda(R)q_\lambda(R)\ . \tag{41}$$

With this convention for the vector dot product we have the same rules for the transformation function, completeness and orthogonality of the basis states, as for the continuous momentum and coordinate dynamical variables of $N\lambda$ components, where N is equal to the total number of lattice points and λ is the total number of bands under consideration. Therefore $N\lambda$ is equal to the dimension of p and q in Eq. (41). Corresponding to Eq. (1) we have

$$\mathscr{H}_{\rm eff}=\left[\frac{1}{\hbar}\right]^{N\lambda}\int d^{N\lambda}p\int d^{N\lambda}q\,H(p,q)\Delta(p,q)\ , \tag{42}$$

where $H(p,q)$ and $\Delta(p,q)$ are given by

$$H(p,q)=\int d^{N\lambda}v\exp\left[\frac{i}{\hbar}p\cdot v\right]\langle q-\tfrac{1}{2}v\,|\,\mathscr{H}\,|\,q+\tfrac{1}{2}v\rangle, \tag{43}$$

$$\Delta(p,q)=\int d^{N\lambda}u\exp\left[\frac{i}{\hbar}q\cdot u\right]|\,p-\tfrac{1}{2}u\rangle\langle p+\tfrac{1}{2}u\,|\ , \tag{44}$$

or by the equivalent expressions

$$H(p,q)=\int d^{N\lambda}u\exp\left[\frac{i}{\hbar}q\cdot u\right]\langle p+\tfrac{1}{2}u\,|\,\mathscr{H}\,|\,p-\tfrac{1}{2}u\rangle\ , \tag{45}$$

$$\Delta(p,q)=\int d^{N\lambda}v\exp\left[\frac{i}{\hbar}p\cdot v\right]|\,q+\tfrac{1}{2}v\rangle\langle q-\tfrac{1}{2}v\,|\ . \tag{46}$$

Corresponding to Eq. (36) we have for the Bose field system

$$\langle q\,|\,U(t,t_0)\,|\,q_0\rangle=\lim_{n\to\infty}\int\cdots\int\prod_{i=1}^{n}d^{N\lambda}q_i\prod_{i=1}^{n+1}\frac{d^{N\lambda}p_i}{\hbar^{N\lambda}}\exp\left\{\frac{i}{\hbar}\sum_{j=1}^{n}(t_j-t_{j-1})\left[p_j\cdot\frac{q_j-q_{j-1}}{t_j-t_{j-1}}-H\left[p_j,\frac{q_j+q_{j-1}}{2}\right]\right]\right\}. \tag{47}$$

Thus there is no difficulty in formulating the path integral for many-boson problems. For a many-particle Bose system $\hat{\pi}=(-\hbar/i)\hat{\phi}^*$ where $\hat{\phi}^*$ is the complex conjugate of $\hat{\phi}$, and hence $p=(-\hbar/i)q^*$.

In order to directly construct the path-integral formulation of many-body fermion (Bloch electron) problems, we have to extend the concept of eigenvalues and eigenvectors to canonical field variables that obey the anticommutation relations.[15,16] Since the fermionic dynamical field operators anticommute, this means that we need a c-number base field of eigenvalues which anticommute (eigenvalues are elements of the Grassmann algebra) rather than the field of ordinary complex numbers. In other words, we will need a quantum representation in terms of external algebra rather than in terms of physical algebra or observables. The elements of this external algebra commute with the elements of the physical algebra or ordinary complex numbers, but anticommute with the canonical field operators. Let us denote the fermionic field operators as $\psi_m^\dagger$ and ψ_r where m and r subsume all indices pertaining to spin, band index, and lattice-point position coordinates. We will assume in what follows that the dimension of ψ^+ and ψ and their eigenvalues is even. Indeed, for the many-body problems considered here, this dimension is even and is equal to $2N\lambda$, where the factor 2 accounts for spin, N is the total number of lattice points, and λ denote the total number of energy bands under consideration.

The canonical field operators satisfy the second quantization or canonical field equations:

$$\{\psi_\alpha,\psi_\beta\}=\{\psi_\alpha^\dagger,\psi_\beta^\dagger\}=0\ , \tag{48}$$

$$\{\psi_\alpha,\psi_\beta^\dagger\}=\delta_{\alpha\beta}\ . \tag{49}$$

The following general eigenvector construction holds for both boson and fermion dynamical operators:[34]

$$|\,q'\rangle=e^{(-i/\hbar)P\cdot q'}\,|\,q'=0\rangle\ , \tag{50}$$

$$\langle p'\,|=\langle p'=0\,|\,e^{(-i/\hbar)p'\cdot Q}\ . \tag{51}$$

For fermions, we substitute $P=i\hbar\psi^\dagger$. Thus for fermions, we have

$$|\,q'\rangle=e^{\psi^\dagger\cdot q'}\,|\,q'=0\rangle,\ \ \psi\,|\,q'=0\rangle=0\ , \tag{52}$$

$$\langle p'\,|=\langle p'=0\,|\,e^{p'\cdot\psi},\ \ \langle p'=0\,|\,\psi^\dagger=0\ , \tag{53}$$

and in addition we also have the following construction:

$$\langle q'\,|=\langle q'=0\,|\,e^{-\psi^\dagger\cdot q'},\ \ \langle q'=0\,|\,\psi=0\ , \tag{54}$$

$$|\,p'\rangle=e^{-p'\cdot\psi}\,|\,p'=0\rangle,\ \ \psi^\dagger\,|\,p'=0\rangle=0\ , \tag{55}$$

where the "dot product" is defined by $\psi^\dagger\cdot q'=\sum_\alpha\psi_\alpha^\dagger q'_\alpha$. In Eqs. (52)—(55), we retained the symbol p and q for the eigenvalues with the understanding that for fermions p

and q are elements of a Grassmann algebra, not ordinary c-numbers. It is important to note that since $\psi^\dagger$ and ψ are non-Hermitian, the operator group generating the eigenvectors is not unitary. Thus, in contrast with boson canonical variables case, for fermions the eigenvector $|0\rangle$, with zero eigenvalue, will acquire a distinguished position in the external quantum-mechanical representation.

Using the identity $e^A B e^{-A} = B + [A,B]$, where the commutator $[A,B]$ is a c-number, one can easily verify that indeed

$$\psi_\alpha^\dagger |p'\rangle = p'_\alpha |p'\rangle = |p'\rangle p'_\alpha , \tag{56}$$

$$\langle p'|\psi_\alpha^\dagger = \langle p'|p'_\alpha = p'_\alpha \langle p'| , \tag{57}$$

$$\psi_\alpha |q'\rangle = q'_\alpha |q'\rangle = |q'\rangle q'_\alpha , \tag{58}$$

$$\langle q'|\psi_\alpha = \langle q'|q'_\alpha = q'_\alpha \langle q'| . \tag{59}$$

Furthermore, we obviously have the following differential operator realizations:

$$\langle p'|\psi = \frac{\vec{\partial}}{\partial p'}\langle p'| = \langle p'| \left[-\frac{\overleftarrow{\partial}}{\partial p'} \right] , \tag{60}$$

$$\psi^\dagger |q'\rangle = \left[-\frac{\vec{\partial}}{\partial q'} \right] |q'\rangle = |q'\rangle \frac{\overleftarrow{\partial}}{\partial q'} , \tag{61}$$

$$\psi |p'\rangle = \left[-\frac{\vec{\partial}}{\partial p'} \right] |p'\rangle = |p'\rangle \frac{\overleftarrow{\partial}}{\partial p'} , \tag{62}$$

$$\langle q'|\psi^\dagger = \frac{\vec{\partial}}{\partial q'}\langle q'| = \langle q'| \left[-\frac{\overleftarrow{\partial}}{\partial q'} \right] , \tag{63}$$

where the arrows denote the left and right derivatives. Using the identity $e^A e^B = e^B e^A e^{[A,B]}$ for the case where the commutator $[A,B]$ is a c-number, we have the following expression for the transformation functions:

$$\langle p'|q'\rangle = e^{p'\cdot q'} = \prod_\alpha e^{p'_\alpha q'_\alpha} = \prod_\alpha (1 + p'_\alpha q'_\alpha) , \tag{64}$$

$$\langle q'|p'\rangle = e^{-p'\cdot q'} = \prod_\alpha (1 + q'_\alpha p'_\alpha) . \tag{65}$$

Using the infinitesimal form of the operator group generating the eigenvectors, Eqs. (52)—(55), one can also deduce the following relations:[34]

$$\langle q'|q''\rangle = (q''_1 - q'_1)(q''_2 - q'_2)\cdots(q''_{2N\lambda} - q'_{2N\lambda}) = \prod_\alpha (q''_\alpha - q'_\alpha) = \delta(q' - q'') , \tag{66}$$

$$\langle p'|p''\rangle = (p'_{2N\lambda} - p''_{2N\lambda})\cdots(p'_1 - p''_1) = \prod_\alpha {}^T(p'_\alpha - p''_\alpha) = \delta(p' - p'') , \tag{67}$$

where the delta function symbol is retained to denote the products of eigenvalue differences. The reason for this is that according to the definition of Grassmann integrals

$$\int d[q']\delta(q' - q'') = \prod_k {}^T \left[\frac{-\vec{\partial}}{\partial q'_k} \right] \prod_k (q''_k - q'_k) = 1 , \tag{68}$$

$$\int d[p']\delta(p' - p'') = \prod_k \left[\frac{\vec{\partial}}{\partial p'_k} \right] \prod_k {}^T(p'_k - p''_k) = 1 . \tag{69}$$

Furthermore, using the resolution of identity given in Appendix B, particular to the external representation, we can derive the following:

$$\langle p'|p''\rangle = \delta(p' - p'') = \int d[q] e^{(p' - p'')\cdot q} , \tag{70}$$

$$\langle q'|q''\rangle = \delta(q' - q'') = \int d[p] e^{-p\cdot(q' - q'')} , \tag{71}$$

where $d[p] \equiv \prod_\alpha dp_\alpha$ represents the volume element in a multidimensional space. Perhaps the above relations are enough to convince the reader that the properties of external representation in terms of eigenvalues defined on a Grassmann algebra are formally identical to that of a quantum representation in terms of boson canonical variables. Other formally identical properties are derived in Appendix B. However, one must bear in mind that integration over anticommuting variables has an entirely different significance, it signifies differentiation with respect to the integration variables. In all mathematical operations, the anticommutation property must be taken into account. The fact that we are dealing with even-dimensional Grassmann variables p and q will greatly simplify the task of taking anticommutation into account.

We have relegated to Appendix B the details of how to directly construct the functional-integral representation of the matrix element of the evolution operator from the underlying external quantum-mechanical representation (c-numbers are elements of the Grassmann algebra). We have also derived the partition function and lattice temperature Green's function as path integrals. The reader is referred to the derivation in Appendix B for the following results. The transition amplitude between a state Ψ specified at time t_0 and a state Φ specified at time t is given by

$$\langle \Phi|\Psi\rangle = \int \prod_{j=1}^{n+1} d[p_j] \prod_{j=0}^{n+1} d[q_j] \phi(q_{n+1}) \exp\left\{ -\epsilon \sum_{j=1}^{n+1} \left[p_j \cdot \frac{q_j - q_{j-1}}{\epsilon} + \frac{i}{\hbar} H\left[p_j, \frac{q_j + q_{j-1}}{2} \right] \right] \right\} \psi(q_0) , \tag{72}$$

where $q_0 = q$ at time t_0, $q_{n+1} = q$ at time $t = t_{n+1}$, and $\epsilon = (t - t_0)/(n+1)$. The wave functions are defined as $\phi(q_{n+1}) = \langle \Phi | q_{n+1}\rangle$ and $\psi(q_0) = \langle q_0 | \Psi\rangle$. $H(p,q)$ is the Weyl transform of the many-body Hamiltonian $\mathcal{H}(\psi^\dagger, \psi)$ and is obtained from $\mathcal{H}(\psi^\dagger, \psi)$ by simple replacement of $\psi^\dagger$ to p and ψ to q. The zero-temperature Green's function is obtained from Eq. (72) by substituting $\Phi = \langle \Psi_0 | e^{(i/\hbar)\mathcal{H}t} \psi_r$ and $\Psi = \psi_s^\dagger e^{(-i/\hbar)\mathcal{H}t_0} | \Psi_0\rangle$ and dividing the result by $i\langle \Psi_0 | \Psi_0\rangle$,

where $|\Psi_0\rangle$ is the ground state of the many-body system. A more useful result is obtained for the grand partition function

$$e^{-\beta\Omega}=\mathrm{Tr}\exp[-\beta(\mathscr{H}-\mu\hat{N})]\equiv\mathrm{Tr}\exp(-\beta\hat{K})\ . \tag{73}$$

We have the expression for the grand partition function given by[17]

$$e^{-\beta\Omega}=\int\prod_{j=1}^{n+1}d[p_j]d[q_j]\exp\left\{-\epsilon\sum_{j=1}^{n+1}\left[p_j\cdot\left[\frac{q_j-q_{j-1}}{\epsilon}\right]+K\left[p_j,\frac{q_j+q_{j-1}}{2}\right]\right]\right\}, \tag{74}$$

where whenever q_0 appears in the action, we take $q_0=-q_{n+1}$. We also have the equivalent expression[18]

$$e^{-\beta\Omega}=\int\prod_{j=0}^{n}d[p_j]d[q_j]\exp\left\{\epsilon\sum_{j=1}^{n+1}\left[\frac{p_j-p_{j-1}}{\epsilon}\cdot q_{j-1}-K\left[\frac{p_j+p_{j-1}}{2},q_{j-1}\right]\right]\right\}, \tag{75}$$

where $\epsilon=\beta/(n+1)$, and whenever p_{n+1} occurs in the action of Eq. (75) we take $p_{n+1}=-p_0$.

Thus the partition function for finite β forces us to define the eigenvalues q and p to be antiperiodic with period β. That the corresponding canonical field operator may also be considered as antiperiodic with period β can be seen from the expression for the finite-temperature Green's function ($\tau>\tau'$).[35] This result can be extended to the "many-operator" Green's function and the antiperiodicity of period β hold for each of the time variables.

The antiperiodic boundary condition on the eigenvalues p and q is precisely what is needed to preserve the antiperiodicity in each of the time variables of the Green's function in the path-integral formulation.[17] Indeed, the finite-temperature Green's function can be written as a path integral:

$$\mathscr{G}_{\alpha\gamma}(\tau,\tau')=-e^{\beta\Omega}\mathrm{Tr}[U(\beta,\tau)\psi_\alpha U(\tau,\tau')\psi_\gamma^\dagger U(\tau',0)]$$

$$=-e^{\beta\Omega}\lim_{\substack{\epsilon\to0\\(n+1)\epsilon=\beta}}\int\prod_{j=1}^{n+1}d[p_j]d[q_j]\exp\left\{-\epsilon\sum_{j=1}^{n+1}\left[p_j\cdot\left[\frac{q_j-q_{j-1}}{\epsilon}\right]+K\left[p_j,\frac{q_j+q_{j-1}}{2}\right]\right]\right\}q_\alpha^\tau p_\gamma^{\tau'} \tag{76}$$

$$=Z^{-1}\int d\mathbf{p}\int d\mathbf{q}\,e^{-S(p,q)}q_\alpha(\tau)p_\gamma(\tau')\ , \tag{77}$$

where

$$\int d\mathbf{p}\int d\mathbf{q}=\lim_{n\to\infty}\int\prod_{j=1}^{n+1}[d^{2N\lambda}p(j)d^{2N\lambda}q(j)]\ ,$$

$Z^{-1}=-e^{\beta\Omega}$, and

$$S(p,q)=\int_0^\beta dt\left\{p(t)\cdot\frac{dq(t)}{dt}+K(p(t),q(t))\right\}. \tag{78}$$

If we denote the right-hand side of Eq. (76) by $\langle q_\alpha^\tau p_\gamma^{\tau'}\rangle$, then it is easy to show that $\langle q_\alpha^\tau\rangle=\langle p_\gamma^\tau\rangle=0$. Physically this is the consequence of the conservation of the number of particles, as this result can also be interpreted as $\langle\psi(\tau)\rangle=\langle\psi^\dagger(\tau)\rangle=0$. The formal definition of the Green's function has been rigorously given by Kato, Kobayashi, and Namiki.[36] The one-particle Green's function is defined as

$$\mathscr{G}_{\alpha\gamma}(\tau,\tau')\equiv\lim_{\eta\to0}\frac{\delta\langle\psi\alpha(\tau)\rangle}{\delta\eta_\gamma(\tau')}\ , \tag{79}$$

where $\eta_\gamma(\tau')$ (also elements of the Grassmann algebra) are components of artificially introduced external sources in the extra symmetry-breaking term added to the Lagrangian of Eq. (78) to have a nonvanishing average value of the field operators; the desired extra term to be added to $S(p,q)$ of Eq. (78) is

$$-\left[\int_0^\beta p\cdot\eta\,dt+\int_0^\beta\eta^\dagger\cdot q\,dt\right], \tag{80}$$

where η and $\eta^\dagger$ are additional anticommuting variables. The right-hand side of Eq. (79) is a functional derivative, but reduces to ordinary differentiation in the discrete-time-step case defined by Eq. (76). Indeed Eq. (79) yields the well-known general formula for the finite-temperature Green's function

$$\mathscr{G}_{\alpha\gamma}(\tau,\tau')\equiv e^{\beta\Omega}\mathrm{Tr}[e^{-\beta\hat{K}}T\psi_\gamma^\dagger(\tau')\psi_\alpha(\tau)]$$

$$\equiv\langle T\psi_\gamma^\dagger(\tau')\psi_\alpha(\tau)\rangle\ , \tag{81}$$

where T stands for the well-known time ordering symbol. The two- and many-particle Green's functions are similarly defined, e.g.,

$$\mathcal{G}_{\alpha\gamma,\delta\mu}(\tau_1\tau_2;\tau_1'\tau_2')=\lim_{\eta\to 0}\frac{\delta^2\langle T\psi_\alpha(\tau_1)\psi_\gamma(\tau_2)\rangle}{\delta\eta_\mu(\tau_1')\delta\eta_\delta(\tau_2')}$$

$$=\langle T\psi_\delta^\dagger(\tau_2')\psi_\mu^\dagger(\tau_1')\psi_\alpha(\tau_1)\psi_\gamma(\tau_2)\rangle\ . \tag{82}$$

All of these Green's functions can be obtained by differentiating (functional derivative in the continuum time limit) the generating functional $G(\eta,\eta^\dagger)$,

$$G(\eta,\eta^\dagger)=e^{\beta\Omega}\int dp\,dq\exp\left[-S(p,q)+\int_0^\beta(p\cdot\eta+\eta^\dagger\cdot q)dt\right], \tag{83}$$

with respect to the external sources η and $\eta^\dagger$ and taking the limit where η and $\eta^\dagger$ go to zero. To complete the discussion on the path-integral formulation of the many-body system, we note from the preceding sections that for a system of fermions and bosons, requiring both commuting and anticommuting dynamical variables for its description, one can similarly construct the path integral by considering product eigenvectors. The generating functional will be of the form

$$G(\eta,\eta^\dagger,J)=Z^{-1}\int dp\int dq\exp\left[-S(p,q,\phi^*,\phi)+\int_0^\beta(\phi\cdot J+p\cdot\eta+\eta^\dagger\cdot q)dt\right], \tag{84}$$

$$S(p,q,\phi)=\int_0^\beta dt\left[p(t)\cdot\frac{dq(t)}{dt}+\phi^*(t)\cdot\frac{d\phi(t)}{dt}-H(p(t),q(t),\phi^*(t),\phi(t))\right], \tag{85}$$

$$Z^{-1}=\int dp\int dq\int d\phi^*\int d\phi\exp[-S(p,q,\phi^*,\phi)]\ . \tag{86}$$

$H(p,q,\phi^*,\phi)$ is obtained from $\mathcal{H}(\psi^\dagger,\psi,\hat\phi^*,\hat\phi)$ by the replacement $\psi^\dagger\to p$, $\psi\to q$, $\hat\phi^*\to\phi^*$, $\hat\phi\to\phi$, with periodic boundary conditions for the boson variables, and antiperiodic boundary conditions for the fermion variables as before, over the length of t equal to β.

We close this section by applying the results obtained here to the many-body Hamiltonian of Eq. (29). We write explicitly the effective Hamiltonian of Eq. (29) (α' and β' do not include spin indices σ):

$$\hat{\mathcal{H}}_{\rm eff}(\psi^\dagger,\psi)=\sum_{\alpha,\beta}\psi_\alpha^\dagger W_{\alpha\beta}^{(1)}\psi_\beta+\sum_{\alpha,\beta}(\psi_\alpha^\dagger\psi_\alpha W_{\alpha\beta}^{(2)c}\psi_\beta^\dagger\psi_\beta-\psi_\alpha^\dagger\psi_\alpha W_{\alpha\beta}^{(2)c}\langle\psi_\beta^\dagger\psi_\beta\rangle_{\rm HF})$$
$$-\sum_{\alpha',\beta',\sigma_1\sigma_2}(\psi_{\alpha'\sigma_1}^\dagger\psi_{\alpha'\sigma_2}W_{\alpha'\beta'\sigma_1\sigma_2}^{(2)\rm ex}\psi_{\beta'\sigma_2}^\dagger\psi_{\beta'\sigma_1}-\psi_{\alpha'\sigma_1}^\dagger\psi_{\alpha'\sigma_2}W_{\alpha'\beta'\sigma_1\sigma_2}^{(2)\rm ex}\langle\psi_{\beta'\sigma_2}^\dagger\psi_{\beta'\sigma_2}\rangle_{\rm HF})\ , \tag{87}$$

where $\langle\cdots\rangle_{\rm HF}$ may be approximated by the Hartree-Fock ground-state average, and from Eqs. (27), (16), and (17),

$$W_{\alpha\beta}^{(1)}=\exp\left[\frac{ie}{\hbar c}A(q_2)\cdot q_1\right]\tilde{\tilde W}_\lambda^{(1)}(q_1-q_2;B)\delta_{\lambda\lambda'}\delta_{\sigma\sigma'}\ , \tag{88}$$

$$W_{\alpha\beta}^{(2)c}=\tilde W_{\lambda_1\lambda_2}^{(2)c}(0,0;2q_1,2q_2;B)\ , \tag{89}$$

$$W_{\alpha'\beta'\sigma_1\sigma_2}^{(2)\rm ex}=\tilde W_{\lambda_1\lambda_2}^{(2)\rm ex}(q_1-q_2,q_2-q_1;q_1+q_2,q_1+q_2;B)\ . \tag{90}$$

The Weyl transform $H(p,q)$ or Weyl symbol (corresponding c-number function) of $\mathcal{H}_{\rm eff}$ is then obtained by replacing $\psi^\dagger$ by p wherever it occurs and similarly substituting q for ψ. We then have $K(p,q)=H(p,q)-\mu p\cdot q$ which can be substituted in all path-integral formulas of this section.

We will not go into the explicit evaluation of the finite-temperature Green's functions describing the dynamics of Bloch electrons as this will lead us far afield. The reader is referred to the work of Sherrington[37] and the references quoted therein for a start in this direction. For practical evaluation of the functional integral using anticommuting variables the reader is referred to some recent interesting work by Samuel.[38] The use of the Grassmann algebra in lattice-gauge-theory calculations is discussed by Wilson[39] and Kadanoff.[40] The use of Monte Carlo methods for evaluating fermionic and coupled boson-fermionic path integrals using a computer has recently emerged as an exciting research activity in the last four years.[41–45]

V. SUMMARY AND CONCLUDING REMARKS

The concept of lattice-space dynamics of electrons in solids may take significant meaning in ultrasubmicron devices and microstructure research, which take advantage of the ever increasing availability of high-speed large-scale computing,[46] as discreteness and/or atomicity in almost all physical quantities of interest begins to dominate the device behavior. In the process of exposing lattice-space dynamics, we have unified various aspects of quantum physics through the Weyl-Wigner formalism of the quantum theory of solids.[20]

Notably, (a) we have generalized, and given a rigorous definition to, the distribution-function operator technique of Brittin and Chappel[47] and that of Klimontovich[48] to particles possessing multiband dynamics (Appendix A); (b) we have incorporated gauge invariance to a universal effective Hamiltonian[31] and indicate how one goes about making a real calculation of deriving the effective Hamiltonian[20–25] (first-stage Weyl transform in external electromagnetic field); (c) we have generalized the method of Soper[17] and Berezin[18] for constructing path integrals and unified their results for the functional-integral expression of the partition function and corresponding finite-temperature Green's function. In Appendix C, we present a simple calculation to demonstrate an applicability of the path-integral technique to the poorly understood very-high-field regime of charge transport in a solid; the "hot-electron Green's function" is analytically calculated for the case where the continuum effective-mass theory is still valid. The result can easily be extended to include scattering by a one-body potential, a problem of interest to submicron device physics. The same application may now further be generalized to the atomistic, or discrete, regime of USER using the formalism developed in this paper.

The first-stage Weyl correspondence essentially enables us to start the quantum-dynamical calculation for nonzero external electromagnetic field from the known zero-field energy band structure. Weyl-Wigner formalism (with built-in mechanism[20–25] for decoupling the band of interest, and yielding a better physical understanding) provides a straightforward approach to establishing isomorphism or Weyl correspondence between operators and c-numbers of the base field, all of which lead to a natural and direct construction of path integrals for single-particle and many-body problems of the lattice-space dynamics of electrons. It is hoped that implementation of the key ideas presented in this paper to problems in USER, ultralarge-scale integration (ULSI) and microstructure science as a whole will take its place with the advent of the scientific-supercomputer age.[46]

It is interesting to note that, already in the past, the interdisciplinary nature of semiconductor solid-state physics and elementary particle physics has appeared explicitly on several occasions in the physics literature. Indeed for a very highly nonparabolic two-band model of some solids (e.g., Bi and Bi-Sb alloys),[32] the nonrelativistic quantum dynamics of Bloch electrons, in an external electromagnetic field, exactly maps onto the theory of fermions in elementary particle physics.[24,25,32] Clearly, path-integral lattice-space dynamics of electrons in solids, as discussed in this paper, bears a very close resemblance to and analogy with lattice gauge theories of elementary particle physics. A further understanding and utilization of the existing analogy could therefore lead to the participation of USER—microstructure-science dynamical problems in the cross-fertilization of ideas between quantum-field theory and statistical mechanics.

A final comment concerning dissipation is in order. Most applications of path integrals are for nondissipative systems. However, the operational nature of the path-integral technique is clearly evident in the construction process. On the other hand, the dissipative aspect of the operational point of view is a property of the process or operation and occurs when the process itself involves a "heat bath" or "nonfunctional" system of a large number of degrees of freedom. That path-integral techniques are naturally capable of treating dissipative systems has indeed been demonstrated by Feynman and Vernon[49] more than two decades ago.

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APPENDIX A: SECOND QUANTIZATION OPERATORS IN SOLID-STATE BAND THEORY

Let $A_{\rm op}^{(1)}$ and $A_{\rm op}^{(2)}$ denote one-body and two-body quantum-mechanical operators, respectively. Following the usual prescription of second quantization procedure we write $A_{\rm op}^{(1)}$ and $A_{\rm op}^{(2)}$ in terms of field operator ψ and its adjoint $\psi^\dagger$ as

$$A_{\rm op}^{(1)}=\int \psi^\dagger(x)A_{\rm op}^{(1)}\psi(x)dx \ , \tag{A1}$$

$$A_{\rm op}^{(2)}=\int\int \psi^\dagger(x)\psi^\dagger(x')A_{\rm op}^{(2)}\psi(x')\psi(x)dx'dx \ . \tag{A2}$$

We decompose the field operators in terms of the Wannier functions:

$$\psi(x)=\sum_{q,\lambda,\sigma}\psi_{\lambda\sigma}(q)\,|\,q,\lambda,\sigma\rangle \ , \tag{A3}$$

$$\psi^\dagger(x)=\sum_{q,\lambda,\sigma}\psi^\dagger_{\lambda\sigma}(q)\langle q,\lambda,\sigma\,| \ . \tag{A4}$$

ψ and $\psi^\dagger$ satisfy the following anticommutation relations:

$$\{\psi_{\lambda\sigma}(q),\psi_{\lambda'\sigma'}(q')\}_+=\{\psi_{\lambda\sigma}(q),\psi_{\lambda'\sigma'}(q')\}=0 \ , \tag{A5}$$

$$\{\psi_{\lambda\sigma}(q),\psi^\dagger_{\lambda'\sigma'}(q')\}=\delta_{q,q'}\delta_{\lambda\lambda'}\delta_{\sigma\sigma'} \ . \tag{A6}$$

Substituting the expression for $A_{\rm op}^{(1)}$ and $A_{\rm op}^{(2)}$ given by Eqs. (1) and (9), respectively, we obtain the following:

$$A_{\rm op}^{(1)}=(N\hbar^3)^{-1}\sum_{p,q,\lambda,\lambda',\sigma,\sigma',v}A^{(1)}_{\lambda\lambda'\sigma\sigma'}(p,q)e^{(2i/\hbar)p\cdot v}\psi^\dagger_{\lambda\sigma}(q+v)\psi_{\lambda'\sigma'}(q-v) \ , \tag{A7}$$

$$A_{\rm op}^{(2)}=(N\hbar^3)^{-2}\sum_{\substack{p,q,\lambda,\lambda',\sigma,\sigma',v,\\ \tilde p,\tilde q,\tilde\lambda,\tilde\lambda',\tilde\sigma,\tilde\sigma',\tilde v}}A^{(2)}_{[\lambda\sigma][\tilde\lambda\tilde\sigma]}(p,\tilde p,q,\tilde q)\exp\left[\frac{2i}{\hbar}(p\cdot v+\tilde p\cdot\tilde v)\right]\psi^\dagger_{\lambda\sigma}(q+v)\psi^\dagger_{\tilde\lambda\tilde\sigma}(\tilde q+\tilde v)\psi_{\tilde\lambda'\tilde\sigma'}(\tilde q-\tilde v)\psi_{\lambda'\sigma'}(q-v) \ . \tag{A8}$$

We can make contact with the work of Brittin and Chappel[47] on the distribution-function operator techniques by rewriting $A_{\rm op}^{(1)}$ and $A_{\rm op}^{(2)}$ as

$$A_{\rm op}^{(1)}=(N\hbar^3)^{-1}\sum_{p,q,\lambda,\lambda',\sigma,\sigma'} A^{(1)}_{\lambda\lambda'\sigma\sigma'}(p,q)\hat{f}^{(1)}_{\lambda\lambda'\sigma\sigma'}(p,q) , \quad \text{(A9)}$$

$$A_{\rm op}^{(2)}=(N\hbar^3)^{-2}\sum_{\substack{p,q,\lambda,\lambda',\sigma,\sigma',\\ \tilde{p},\tilde{q},\tilde{\lambda},\tilde{\lambda}',\tilde{\sigma},\tilde{\sigma}'}} A^{(2)}_{[\lambda\sigma][\tilde{\lambda}\tilde{\sigma}]}(p,\tilde{p},q,\tilde{q}) \times\hat{f}^{(2)}_{[\lambda\sigma][\tilde{\lambda}\tilde{\sigma}]}(p,\tilde{p},q,\tilde{q}) , \quad \text{(A10)}$$

where

$$\hat{f}^{(1)}_{\lambda\lambda'\sigma\sigma'}(p,q)=\sum_{v} e^{(2i/\hbar)p\cdot v}\psi^{\dagger}_{\lambda\sigma}(q+v)\psi_{\lambda'\sigma'}(q-v) , \quad \text{(A11)}$$

$$\hat{f}^{(2)}_{[\lambda\sigma][\tilde{\lambda}\tilde{\sigma}]}(\tilde{p},p,\tilde{q},q) =\sum_{v,\tilde{v}}\exp\left[\frac{2i}{\hbar}(p\cdot\tilde{v}+\tilde{p}\cdot v)\right]\psi^{\dagger}_{\lambda\sigma}(q+v)\psi^{\dagger}_{\tilde{\lambda}\tilde{\sigma}}(\tilde{q}+\tilde{v}) \times\psi_{\tilde{\lambda}'\tilde{\sigma}'}(\tilde{q}-\tilde{v})\psi_{\lambda'\sigma'}(q-v) . \quad \text{(A12)}$$

We can now see that the quantities $\hat{f}^{(1)}_{\lambda\lambda'\sigma\sigma'}(p,q)$ and $\hat{f}^{(2)}_{[\lambda\sigma][\tilde{\lambda}\tilde{\sigma}]}(p,\tilde{p},q,\tilde{q})$ given above for solid-state band theory correspond to the Klimontovich[48] second quantization operator for one- and two-particle [interacting free particles, not interacting Bloch particles to which Eqs. (A11) and (A12) generally apply] phase-space distribution functions, respectively, which were also obtained by Brittin and Chappell.[47] Our band-theory result essentially differs from that of Klimontovich[48] and Brittin and Chappell[47] by replacement of integration by summation and the absence of "half-displacements" of the field operators. Brittin and Chappell have shown that the expectation value of $\hat{f}^{(1)}(p,q)$ which we will denote by $\langle f^{(1)}(p,q)\rangle$ is equal to the Wigner distribution function, which is shown here to be the lattice Weyl transform, Eq. (2), of the density-matrix operator. In the solid-state band-theory case, using arguments analogous to those given by Brittin and Chappell one can easily verify that indeed,

$$\langle f^{(1)}_{\lambda\lambda'\sigma\sigma'}(p,q)\rangle=\rho^{(1)}_{\lambda'\lambda\sigma'\sigma}(p,q) , \quad \text{(A13)}$$

where the right-hand side of Eq. (A13) is the lattice Weyl transform [Eq. (2)] of the density-matrix operator $\hat{\rho}^{(1)}$,

$$\rho^{(1)}_{\lambda'\lambda\sigma'\sigma}(p,q) =\sum_{v}\exp\left[\frac{2i}{\hbar}p\cdot v\right]\langle q-v,\lambda',\sigma'\,|\,\hat{\rho}^{(1)}\,|\,q+v,\lambda,\sigma\rangle , \quad \text{(A14)}$$

and $\hat{\rho}^{(1)}$ is the one-particle density-matrix operator. Similarly, we have

$$\langle\hat{f}^{(2)}_{[\lambda\sigma][\tilde{\lambda}\tilde{\sigma}]}(p,\tilde{p},q,\tilde{q})\rangle=\rho^{(2)}_{[\lambda\sigma][\tilde{\lambda}\tilde{\sigma}]^T}(p,\tilde{p},q,\tilde{q}) , \quad \text{(A15)}$$

where $[\lambda\sigma][\tilde{\lambda}\tilde{\sigma}]^T$ stands for $\lambda'\sigma'\lambda\sigma\tilde{\lambda}'\tilde{\sigma}'\tilde{\lambda}\tilde{\sigma}$ and the right-hand side of Eq. (A15) is the lattice Weyl transform of the two-particle density-matrix operator $\hat{\rho}^{(2)}$,

$$\rho^{(2)}_{[\lambda\sigma][\tilde{\lambda}\tilde{\sigma}]^T}(p,\tilde{p},q,\tilde{q}) =\sum_{v,\tilde{v}}\exp\left[\frac{2i}{\hbar}(p\cdot v+\tilde{p}\cdot\tilde{v})\right]\langle q-v,\lambda',\sigma'\,|\,\langle\tilde{q}-\tilde{v},\tilde{\lambda}'\tilde{\sigma}'\,| \times\hat{\rho}^{(2)}\,|\,\tilde{q}+\tilde{v},\tilde{\lambda},\tilde{\sigma}\rangle\,|\,q+v,\lambda,\sigma\rangle . \quad \text{(A16)}$$

The expectation value of $A_{\rm op}^{(1)}$ and $A_{\rm op}^{(2)}$, Eqs. (A9) and (A10), respectively, is thus given by

$$\langle A_{\rm op}^{(1)}\rangle=\sum_{p,q,\lambda,\lambda',\sigma,\sigma'} A^{(1)}_{\lambda\lambda'\sigma\sigma'}(p,q)\rho^{(1)}_{\lambda'\lambda\sigma'\sigma}(p,q) , \quad \text{(A17)}$$

$$\langle A_{\rm op}^{(2)}\rangle=\sum_{\substack{p,q,\lambda,\lambda',\sigma,\sigma',\\ \tilde{p},\tilde{q},\tilde{\lambda},\tilde{\lambda}',\tilde{\sigma},\tilde{\sigma}'}} A^{(2)}_{[\lambda\sigma][\tilde{\lambda}\tilde{\sigma}]}(p,\tilde{p},q,\tilde{q}) \times\rho^{(2)}_{[\lambda\sigma][\tilde{\lambda}\tilde{\sigma}]^T}(p,\tilde{p},q,\tilde{q}) . \quad \text{(A18)}$$

Equations (A17) and (A18) calculate quantum-mechanical averages in exactly the same manner as calculating classical-mechanical averages using the phase-space distribution function. However, some differences in the quantities involved must be noted. For multiband particles $A^{(1)}_{\lambda\lambda'\sigma\sigma'}(p,q)$ and $A^{(2)}_{[\lambda\sigma][\tilde{\lambda}\tilde{\sigma}]}(p,\tilde{p},q,\tilde{q})$ which are the lattice Weyl transforms of $A_{\rm op}^{(1)}$ and $A_{\rm op}^{(2)}$, respectively, do not in general resemble any of the dynamical expressions in classical mechanics, since they are in general, functions of $\hbar$, Planck's constant divided by 2π. Moreover, the method employed here to derive Eqs. (A9) and (A10) is quite rigorous as compared to the ansatz employed by Brittin and Chappell[47] to derive Eqs. (III.35) and (III.36) of their paper. The classical functions contemplated in their equations are limiting cases of the general classical functions (Weyl transforms) used in Eqs. (A9) and (A10) of this paper, in the limit that the crystal lattice points form a continuum and there is only one band. For some interesting applications of the distribution-function operator technique to equilibrium and nonequilibrium problems, the readers are referred to Refs. 48, 50, and 51.

Solutions to problems in solid-state physics often start by writing down the effective Hamiltonian.[21,31] However, the writing down of a correct (good approximation to the problem at hand) effective Hamiltonian usually hinges on one's intuition and experience. We will give a rigorous derivation of a universal effective Hamiltonian for Bloch particles through the first-stage Weyl correspondence discussed in Sec. II. We will cast the effective Hamiltonian of a many-body problem which we assumed to be a sum of one- and two-body operators, Eqs. (A9) and (A10), respectively, in a form that is more familiar and most amenable to field-theoretical perturbation techniques. First we derive the effective second quantization one- and two-body operators in lattice coordinate space. This is immediately done by carrying out the summation over the (momentum) variables in Eqs. (A7) and (A8). The result is

$$A_{\rm op}^{(1)}=\sum_{q,v,\lambda,\lambda',\sigma,\sigma'} W_{\lambda\lambda'\sigma\sigma'}^{(1)}(2v,2q)\psi_{\lambda\sigma}^{\dagger}(q+v)\psi_{\lambda'\sigma'}(q-v)\ , \tag{A19}$$

$$A_{\rm op}^{(2)}=\sum_{\substack{q,v,\lambda,\lambda',\sigma,\sigma',\\ \tilde{q},\tilde{v},\tilde{\lambda},\tilde{\lambda}',\tilde{\sigma},\tilde{\sigma}'}} W_{[\lambda\sigma][\tilde{\lambda}\tilde{\sigma}]}^{(2)}(2v,2\tilde{v},2q,2\tilde{q}) \times\psi_{\lambda\sigma}^{\dagger}(q+v)\psi_{\tilde{\lambda}\tilde{\sigma}}^{\dagger}(\tilde{q}+\tilde{v}) \times\psi_{\tilde{\lambda}'\tilde{\sigma}'}(\tilde{q}-\tilde{v})\psi_{\lambda'\sigma'}(q-v)\ , \tag{A20}$$

where we have defined

$$W_{\lambda\lambda'\sigma\sigma'}^{(1)}(2v,2q)=\sum_{p} e^{(2i/\hbar)p\cdot v}A_{\lambda\lambda'\sigma\sigma'}(p,q)\ , \tag{A21}$$

$$W_{[\lambda\sigma][\tilde{\lambda}\tilde{\sigma}]}^{(2)}(2v,2\tilde{v},2q,2\tilde{q}) =\sum_{p,\tilde{p}}\exp\left[\frac{2i}{\hbar}(p\cdot v+\tilde{p}\cdot\tilde{v})\right]A_{[\lambda\sigma][\tilde{\lambda}\tilde{\sigma}]}^{(2)}(p,\tilde{p},q,\tilde{q})\ . \tag{A22}$$

A more transparent form is obtained by transforming the lattice coordinate variables involved in the summation and writing

$$A_{\rm op}^{(1)}=\sum_{R_1,R_2,\lambda,\lambda',\sigma,\sigma'} W_{\lambda\lambda'\sigma\sigma'}^{(1)}(R_1-R_2;R_1+R_2)\psi_{\lambda\sigma}^{\dagger}(R_1)\psi_{\lambda'\sigma'}(R_2)\ , \tag{A23}$$

$$A_{\rm op}^{(2)}=\sum_{\substack{R_1,R_2,\lambda,\lambda',\sigma,\sigma',\\ \tilde{R}_1,\tilde{R}_2,\tilde{\lambda},\tilde{\lambda}',\tilde{\sigma},\tilde{\sigma}'}} W_{[\lambda\sigma][\tilde{\lambda}\tilde{\sigma}]}^{(2)}(R_1-R_2,\tilde{R}_1-\tilde{R}_2;R_1+R_2,\tilde{R}_1+\tilde{R}_2)\psi_{\lambda\sigma}^{\dagger}(R_1)\psi_{\tilde{\lambda}\tilde{\sigma}}^{\dagger}(\tilde{R}_1)\psi_{\tilde{\lambda}'\tilde{\sigma}'}(\tilde{R}_2)\psi_{\lambda'\sigma'}(R_2)\ . \tag{A24}$$

It is easy to show by using Eqs. (2) and (A21), and Eqs. (10) and (A22), that indeed

$$W_{\lambda\lambda'\sigma\sigma'}^{(1)}(R_1-R_2;R_1+R_2)=\langle R_1,\lambda,\sigma\,|\,A_{\rm op}^{(1)}\,|\,R_2,\lambda',\sigma'\rangle\ , \tag{A25}$$

$$W_{[\lambda\sigma][\tilde{\lambda}\tilde{\sigma}]}^{(2)}(R_1-R_2,\tilde{R}_1-\tilde{R}_2;R_1+R_2,\tilde{R}_1+\tilde{R}_2) =\langle R_1\lambda\sigma\,|\,\langle\tilde{R}_1\tilde{\lambda}\tilde{\sigma}\,|\,A_{\rm op}^{(2)}\,|\,\tilde{R}_2\tilde{\lambda}'\tilde{\sigma}'\rangle\,|\,R_2\lambda'\sigma'\rangle\ , \tag{A26}$$

as one would expect from the form of Eqs. (A23) and (A24). Our result also shows that $W^{(1)}$ and $W^{(2)}$ are functions of the sum and difference of lattice-point coordinates only.

To derive the effective one- and two-body operators in p (momentum) space we lattice-Fourier-transform the field operator in q (lattice coordinate) space to the p (momentum) space:

$$\psi_{\alpha}^{\dagger}(q+\nu)=(N\hbar^3)^{-1/2}\sum_{p}\exp\left[-\frac{ip}{\hbar}\cdot(q+v)\right]a_{\alpha}^{\dagger}(p)\ , \tag{A27}$$

$$\psi_{\beta}(q-\nu)=(N\hbar^3)^{-1/2}\sum_{p}\exp\left[\frac{ip}{\hbar}\cdot(q-v)\right]a_{\beta}(p)\ . \tag{A28}$$

The equivalent expression for the one- and two-particle distribution-function operators $\hat{f}^{(1)}$ and $\hat{f}^{(2)}$ can thus be written as

$$\hat{f}_{\lambda\lambda'\sigma\sigma'}^{(1)}(p,q)=\sum_{u}\exp\left[\frac{2i}{\hbar}u\cdot q\right]a_{\lambda\sigma}^{\dagger}(p-u)a_{\lambda'\sigma'}(p+u)\ , \tag{A29}$$

$$\hat{f}_{[\lambda\sigma][\tilde{\lambda}\tilde{\sigma}]}^{(2)}(p,\tilde{p},q,\tilde{q}) =\sum_{u,\tilde{u}}\exp\left[\frac{2i}{\hbar}(q\cdot u+\tilde{q}\cdot\tilde{u})\right]a_{\lambda\sigma}^{\dagger}(p-u) \times a_{\tilde{\lambda}\tilde{\sigma}}^{\dagger}(\tilde{p}-\tilde{u})a_{\tilde{\lambda}'\tilde{\sigma}'}(\tilde{p}+\tilde{u})a_{\lambda'\sigma'}(p+u)\ . \tag{A30}$$

Substituting the last two equations in Eqs. (A9) and (A10), we obtain

$$A_{\rm op}^{(1)}=\sum_{p,u,\lambda,\lambda',\sigma,\sigma'} W_{\lambda\lambda'\sigma\sigma'}^{(1)}(2p,2u) \times a_{\lambda\sigma}^{\dagger}(p-u)a_{\lambda'\sigma'}(p+u)\ , \tag{A31}$$

$$A_{\rm op}^{(2)}=\sum_{\substack{p,u,\lambda,\lambda',\sigma,\sigma',\\ \tilde{p},\tilde{u},\tilde{\lambda},\tilde{\lambda}',\tilde{\sigma},\tilde{\sigma}'}} W_{[\lambda\sigma][\tilde{\lambda}\tilde{\sigma}]}^{(2)}(2p,2\tilde{p},2u,2\tilde{u}) \times a_{\lambda\sigma}^{\dagger}(p-u)a_{\tilde{\lambda}\tilde{\sigma}}^{\dagger}(\tilde{p}-\tilde{u}) \times a_{\tilde{\lambda}'\tilde{\sigma}'}(\tilde{p}+\tilde{u})a_{\lambda'\sigma'}(p+u)\ , \tag{A32}$$

where

$$W_{\lambda\lambda'\sigma\sigma'}^{(1)}(2p,2u)=\sum_{q}\exp\left[\frac{2i}{\hbar}u\cdot q\right]A_{\lambda\lambda'\sigma\sigma'}^{(1)}(p,q)\ , \tag{A33}$$

$$W_{[\lambda\sigma][\tilde{\lambda}\tilde{\sigma}]}^{(2)}(2p,2\tilde{p};2u,2\tilde{u}) =\sum_{q,\tilde{q}}\exp\left[\frac{2i}{\hbar}(u\cdot q+\tilde{u}\cdot\tilde{q})\right]A_{[\lambda\sigma][\tilde{\lambda}\tilde{\sigma}]}^{(2)}(p,\tilde{p},q,\tilde{q})\ . \tag{A34}$$

A familiar second quantization form in p (momentum or wave vector) space is again obtained by transforming the momentum variables involved in the summation to yield

$$A_{\rm op}^{(1)}=\sum_{k_1,k_2,\lambda,\lambda',\sigma,\sigma'} W^{(1)}_{\lambda\lambda'\sigma\sigma'}(k_1+k_2;k_2-k_1) \times a^{\dagger}_{\lambda\sigma}(k_1)a_{\lambda'\sigma'}(k_2)\ , \tag{A35}$$

$$A_{\rm op}^{(2)}=\sum_{\substack{k_1,k_2,\lambda,\lambda',\sigma,\sigma',\\ \tilde{k}_1,\tilde{k}_2,\tilde{\lambda},\tilde{\lambda}',\tilde{\sigma},\tilde{\sigma}'}} W^{(2)}_{[\lambda\sigma][\tilde{\lambda}\tilde{\sigma}]} \times(k_1+k_2,\tilde{k}_1+\tilde{k}_2;k_2-k_1,\tilde{k}_1-\tilde{k}_1) \times a^{\dagger}_{\lambda\sigma}(k_1)a^{\dagger}_{\tilde{\lambda}\tilde{\sigma}}(\tilde{k}_1)a_{\tilde{\lambda}'\tilde{\sigma}'}(\tilde{k}_2)a_{\lambda'\sigma'}(k_2)\ , \tag{A36}$$

where again one can easily show that

$$W^{(1)}_{\lambda\lambda'\sigma\sigma'}(k_1+k_2;k_2-k_1)=\langle k,\lambda\sigma\,|\,A^{(1)}_{\rm op}\,|\,k_2\lambda'\sigma'\rangle\ , \tag{A37}$$

$$W^{(2)}_{[\lambda\sigma][\tilde{\lambda}\tilde{\sigma}]}(k_1+k_2,\tilde{k}_1+\tilde{k}_2;k_2-k_1,\tilde{k}_2-\tilde{k}_1) =\langle k_1\lambda\sigma\,|\,\langle\tilde{k}_1\tilde{\lambda}\tilde{\sigma}\,|\,A^{(2)}_{\rm op}\,|\,\tilde{k}_2\tilde{\lambda}'\tilde{\sigma}'\rangle\,|\,k_2\lambda'\sigma'\rangle\ , \tag{A38}$$

as expected. The virtue of the calculation presented here is that it explicitly shows the functional dependence of the matrix elements, entirely quantum-mechanical quantities, and their exact relation to the lattice Weyl transform of the corresponding operators through the defining relations, Eqs. (2), (4), and (10), and its equivalent expression (A21), (A22), (A33), and (A34).

APPENDIX B: DIRECT CONSTRUCTION OF FERMIONIC PATH INTEGRAL

We will generalize the method and unify the results of Soper[17] and Berezin[18] to construct the path-integral forms given in the text. We make use of the eigenvectors construction given by Eqs. (52)—(55). The reader is referred to Ref. 34 for the notations used here. The basic idea is to formulate the Weyl correspondence[23] in the external representation of fermions. We will need the following theorems.

Theorem 1. Resolution of identity in the external representation is given by

$$\begin{aligned}1&=\exp\left[\psi^{\dagger}\cdot\frac{\vec{\partial}}{\partial p'}\right]\,|\,q'=0\rangle\langle p'=0\,|\,e^{p'\cdot\psi}\\ &=e^{\psi^{\dagger}\cdot q'}\,|\,q'=0\rangle\langle p'=0\,|\exp\left[\frac{\overleftarrow{\partial}^{T}}{\partial q'}\cdot\psi\right]\\ &=\exp\left[-\frac{\vec{\partial}}{\partial q'}\cdot\psi\right]\,|\,p'=0\rangle\langle q'=0\,|\,e^{-\psi^{\dagger}\cdot q'}\\ &=e^{-p'\cdot\psi}\,|\,p'=0\rangle\langle q'=0\,|\exp\left[-\psi^{\dagger}\cdot\frac{\overleftarrow{\partial}^{T}}{\partial p'}\right]\ .\end{aligned} \tag{B1}$$

The proof can be shown by comparison with[19]

$$1=|\,p'=0\rangle\langle q'=0\,|+\psi_r\,|\,p'=0\rangle\langle q'=0\,|\,\psi_r^{\dagger}+\cdots \tag{B2}$$

$$=|\,q'=0\rangle\langle p'=0\,|+\psi_r^{\dagger}\,|\,q'=0\rangle\langle p'=0\,|\,\psi_r+\cdots\ . \tag{B3}$$

Corollary 1.1. In terms of the q eigenvectors only or in terms of p eigenvectors only, we have the following expression for completeness:

$$1=|\,q'\rangle\left\langle\frac{\overleftarrow{\partial}^{T}}{\partial q'}\,\middle|\,\frac{\vec{\partial}}{\partial q''}\right\rangle\langle q''\,| \tag{B4}$$

$$=|\,p'\rangle\left\langle\frac{\overleftarrow{\partial}^{T}}{\partial p'}\,\middle|\,\frac{\vec{\partial}}{\partial p''}\right\rangle\langle p''\,|\ . \tag{B5}$$

Corollary 1.2. The scalar product in the q representation is given by

$$\begin{aligned}\langle\phi\,|\,\psi\rangle&=\phi(q')\left\langle\frac{\overleftarrow{\partial}^{T}}{\partial q'}\,\middle|\,\frac{\vec{\partial}}{\partial q''}\right\rangle\psi(q'')\\ &=\phi(q')\Pi^{T}\left[\frac{\overleftarrow{\partial}^{T}}{\partial q'}-\frac{\vec{\partial}}{\partial q''}\right]\psi(q'')\\ &=\Pi^{T}-\left[\frac{\vec{\partial}}{\partial q'}+\frac{\vec{\partial}}{\partial q''}\right]\phi(q')\psi(q'')\\ &=\Pi^{T}\left[-\frac{\partial}{\partial q}\right]\phi(q)\psi(q)=\Pi^{T}\left[\frac{\partial}{\partial q}\right]\phi(q)\psi(q)\\ &=\int d[q]\phi(q)\psi(q)\ ,\end{aligned} \tag{B6}$$

and similarly in the p representation.

Theorem 2. For any operator A, we have

$$\langle p'\,|\,A_{\rm op}\,|\,q'\rangle\left\langle\frac{\overleftarrow{\partial}^{T}}{\partial q'}\,\middle|\,\frac{\overleftarrow{\partial}^{T}}{\partial p'}\right\rangle =\int d[q']d[p']e^{p'\cdot q'}\langle p'\,|\,A_{\rm op}\,|\,q'\rangle\ . \tag{B7}$$

Proof:

$$\begin{aligned}{\rm Tr}A_{\rm op}&=\left\langle p'\,\middle|\,A_{\rm op}\,\middle|\,\frac{\overleftarrow{\partial}^{T}}{\partial p'}\right\rangle=\langle p'\,|\,A_{\rm op}\,|\,q'\rangle\left\langle\frac{\overleftarrow{\partial}^{T}}{\partial q'}\,\middle|\,\frac{\overleftarrow{\partial}^{T}}{\partial p'}\right\rangle\\ &=\left\langle\frac{\vec{\partial}}{\partial q'}\,\middle|\,\frac{\vec{\partial}}{\partial p'}\right\rangle\langle p'\,|\,A_{\rm op}\,|\,q'\rangle\ .\end{aligned} \tag{B8}$$

But ${\rm Tr}A_{\rm op}$ is also given by[34]

$$\begin{aligned}\mathrm{Tr}A_{\mathrm{op}} &= \int d[q']d[p']e^{p'\cdot q'}\langle p' \mid A_{\mathrm{op}} \mid q'\rangle \\ &= \int d[q']d[p']e^{p'\cdot q'}\langle p'=0 \mid [1+(p\cdot\psi)+\cdots]A_{\mathrm{op}}[1+(\psi^{\dagger}\cdot q)+\cdots] \mid q'=0\rangle \\ &= \langle p'=0 \mid A_{\mathrm{op}} \mid q'=0\rangle + \langle p'=0 \mid \psi_r A_{\mathrm{op}}\psi_r^{\dagger} \mid q'=0\rangle + \cdots \end{aligned} \tag{B9}$$

and therefore the theorem is proved.

Corollary 2.1. The expression for completeness in the p-q mixed representation is given symbolically by

$$1 = \int d[q']d[p']e^{-p'\cdot q'} \mid q'\rangle\langle p' \mid . \tag{B10}$$

Proof:

$$1 = \mid q'\rangle\left\langle \frac{\overleftarrow{\partial}^{T}}{\partial q'} \middle| \frac{\vec{\partial}}{\partial p'}\right\rangle\langle p' \mid = \left\langle -\frac{\vec{\partial}}{\partial q'} \middle| \frac{\vec{\partial}}{\partial p'}\right\rangle \mid q'\rangle\langle p' \mid$$

$$= \int d[q']d[p']e^{-p'\cdot q'} \mid q'\rangle\langle p' \mid . \tag{B11}$$

The last result is the completeness relation used by Halpern, Jevicki, and Senjanovic[19] for constructing fermionic path integrals, which was later generalized by Soper.[17]

We will now establish the Weyl correspondence. We make use of the following identity for an arbitrary operator A:

$$A = \mid q''\rangle\left\langle \frac{\overleftarrow{\partial}^{T}}{\partial q''} \middle| \frac{\vec{\partial}}{\partial p''}\right\rangle\langle p'' \mid A \mid p'\rangle\left\langle \frac{\overleftarrow{\partial}^{T}}{\partial p'} \middle| \frac{\vec{\partial}}{\partial q'}\right\rangle\langle q' \mid \tag{B12}$$

$$= \int d[q'']d[p'']d[q']d[p']e^{-p''\cdot q''+p'\cdot q'} \times \mid q''\rangle\langle p'' \mid A \mid p'\rangle\langle q' \mid , \tag{B13}$$

where the last line is obtained using corollary 2.1. Introducing the change of variables

$$p'=p-u,\quad q'=q-v\ , \qquad p''=p+u,\quad q''=q+v\ , \tag{B14}$$

we obtain

$$A = \int d[q]d[p]A(p,q)\Delta(p,q)\ , \tag{B15}$$

where

$$A(p,q) = \int d[u]e^{-2u\cdot q}\langle p+u \mid A \mid p-u\rangle\ , \tag{B16}$$

$$\Delta(p,q) = \int d[v]e^{-2p\cdot v} \mid q+v\rangle\langle q-v \mid . \tag{B17}$$

$A(p,q)$, which is a c-number quantity, represents the Weyl transform of an arbitrary operator A and (B16) is the realization of Weyl correspondence in the external algebra representation. One can show using the differential operator realization of Eqs. (60)—(63) and the properties of the delta function in the external representation that indeed $A(p,q)$ can be obtained from the operator $A(\psi^{\dagger},\psi)$ by replacement as $\psi^{\dagger}\to p$ and $\psi\to q$. One can easily check the consistency of the expression (B15) by calculating the trace of A. From (B9) we have

$$\begin{aligned}\mathrm{Tr}A &= \int d[q']\int d[p']e^{p'\cdot q'}\langle p' \mid A \mid q'\rangle \\ &= \int d[q]\int d[p]A(p,q)\delta(p)\delta(q)e^{-2p\cdot q} \\ &= \int d[u]\langle u \mid A \mid -u\rangle\ . \end{aligned} \tag{B18}$$

The last line of Eq. (B18) can indeed be shown to be the variant expression for the trace of an arbitrary operator specific to the external algebra representation.[34] To show this one makes use of the form of Eq. (B7) using only q variables.

We note that an arbitrary operator A can also be expressed in the form which is a variant of Eq. (B12),

$$A = \mid p''\rangle\left\langle \frac{\overleftarrow{\partial}^{T}}{\partial p''} \middle| \frac{\vec{\partial}}{\partial q''}\right\rangle\langle q'' \mid A \mid q'\rangle\left\langle \frac{\overleftarrow{\partial}^{T}}{\partial q'} \middle| \frac{\vec{\partial}}{\partial p'}\right\rangle\langle p' \mid$$

$$= \int d[q]\int d[p]A(p,q)\tilde{\Delta}(p,q)\ , \tag{B19}$$

where

$$A(p,q) = \int d[v]e^{2p\cdot v}\langle q+v \mid A \mid q-v\rangle\ , \tag{B20}$$

$$\tilde{\Delta}(p,q) = \int d[u]e^{2u\cdot q} \mid p+u\rangle\langle p-u \mid . \tag{B21}$$

We are now in the position to calculate the path-integral expression of the evolution operator

$$U(t,t_0) = e^{-(i/\hbar)(t-t_0)\mathscr{H}} = \prod_{j=1}^{n+1} U(t_j,t_{j-1}) \mid_{t_0=t_0}^{t_{n+1}=t}\ . \tag{B22}$$

Using the resolution of identity (theorem 1) we have

$$U(t,t_0) = \mid q_{n+1}\rangle\left\langle \frac{\overleftarrow{\partial}^{T}}{\partial q_{n+1}} \middle| \left[\prod_{j=1}^{n+1} \middle| \frac{\vec{\partial}}{\partial q_j}\right\rangle\langle q_j \mid U(t_j,t_{j-1}) \mid q_{j-1}\rangle\left\langle \frac{\overleftarrow{\partial}^{T}}{\partial q_{j-1}} \middle| \right]\middle| \frac{\vec{\partial}}{\partial q_0}\right\rangle\langle q_0 \mid , \tag{B23}$$

or the equivalent expression

$$U(t,t_0) = \mid p_{n+1}\rangle\left\langle \frac{\overleftarrow{\partial}^{T}}{\partial p_{n+1}} \middle| \left[\prod_{j=1}^{n+1} \middle| \frac{\vec{\partial}}{\partial p_j}\right\rangle\langle p_j \mid U(t_j,t_{j-1}) \mid p_{j-1}\rangle\left\langle \frac{\overleftarrow{\partial}^{T}}{\partial p_{j-1}} \middle| \right]\middle| \frac{\vec{\partial}}{\partial p_0}\right\rangle\langle p_0 \mid . \tag{B24}$$

It will be convenient to use the representation of an arbitrary operator given by Eqs. (B15)—(B17) in evaluating the products in Eq. (B23) and similarly the representation of Eqs. (B19)—(B21) in evaluating the products of Eq. (B24). We have from (B17) and (B23), making use of Eq. (66), the following:

$$\begin{aligned}\langle q_j \mid \Delta(p,q) \mid q_{j-1}\rangle &= \int d[v] e^{-2p\cdot v}\langle q_j \mid q+v\rangle\langle q-v \mid q_{j-1}\rangle \\ &= \int d[v] e^{-2p\cdot v}\prod_\alpha (q^\alpha+v^\alpha-q_j^\alpha)\prod_\gamma (q_{j-1}^\gamma-q^\gamma+v^\gamma) \\ &= \int d[v] e^{-2p\cdot v}\prod_\alpha [2v^\alpha-(q_j^\alpha-q_{j-1}^\alpha)]\prod_\gamma [q^\gamma-(q_{j-1}^\gamma+q_j^\gamma)/2] \\ &= e^{-p\cdot(q_j-q_{j-1})}\delta\left[\frac{q_{j-1}+q_j}{2}-q\right] . \end{aligned} \tag{B25}$$

By virtue of Eqs. (B15) and (B22) we may then write, correct to order $(t_j-t_{j-1})^2$,

$$\langle q_j \mid U(t_j,t_{j-1}) \mid q_{j-1}\rangle = \int d[p] e^{-p\cdot(q_j-q_{j-1})}\exp\left[-\frac{i}{\hbar}(t_j-t_{j-1})H\left[p,\frac{q_j+q_{j-1}}{2}\right]\right] . \tag{B26}$$

With the aid of corollaries 1.1 and 1.2, we can symbolically write

$$U(t,t_0)=\int\prod_{j=1}^{n+1} d[p_j]\int\prod_{j=0}^{n+1} d[q_j]\mid q_{n+1}\rangle\exp\left\{-\epsilon\sum_{j=1}^{n+1}\left[p_j\cdot\frac{q_j-q_{j-1}}{\epsilon}+\frac{1}{\hbar}H\left[p_j,\frac{q_j+q_{j-1}}{2}\right]\right]\right\}\langle q_0 \mid . \tag{B27}$$

Similarly the use of Eq. (B24) together with Eqs. (B19)—(B21) yield the equivalent expression

$$U(t,t_0)=\int\prod_{j=0}^{n+1} d[p_j]\int\prod_{j=0}^{n} d[q_j]\mid p_{n+1}\rangle\exp\left\{\epsilon\sum_{j=1}^{n+1}\left[\frac{p_j-p_{j-1}}{\epsilon}\cdot q_{j-1}-\frac{i}{\hbar}H\left[\frac{p_j+p_{j-1}}{2},q_{j-1}\right]\right]\right\}\langle p_0 \mid . \tag{B28}$$

Using the expression for the trace given by Eq. (B18), we have from Eq. (B27)

$$\mathrm{Tr}\,U(t,t_0)=\int\prod_{j=1}^{n+1} d[p_j]\int\prod_{j=0}^{n+1} d[q_j]\delta(q_0+q_{n+1})\exp\left\{-\epsilon\sum_{j=1}^{n+1}\left[p_j\cdot\frac{q_j-q_{j-1}}{\epsilon}+\frac{i}{\hbar}H\left[p_j,\frac{q_j-q_{j-1}}{2}\right]\right]\right\} , \tag{B29}$$

which upon integrating over $d[q_0]$ leads to Eq. (74) for the grand partition function, with antiperiodic boundary conditions on q resulting from the Kronecker delta function in Eq. (B29). Equation (74) corresponds to the result given by Soper.[17] Similarly taking the trace of the expression in Eq. (B28) yields the equivalent expression for the trace of $U(t,t_0)$,

$$\mathrm{Tr}\,U(t,t_0)=\int\prod_{j=0}^{n+1} d[p_j]\int\prod_{j=0}^{n} d[q_j]\delta(p_0+p_{n+1})\exp\left\{\epsilon\sum_{j=1}^{n+1}\left[\frac{p_j-p_{j-1}}{\epsilon}\cdot q_{j-1}-\frac{i}{\hbar}H\left[\frac{p_j+p_{j-1}}{2},q_{j-1}\right]\right]\right\} , \tag{B30}$$

which upon integrating over $d[p_{n+1}]$ leads to Eq. (75) for the grand partition function, with antiperiodic boundary conditions on p resulting from the Kronecker delta function in Eq. (B30). Equation (75) corresponds to the result given by Berezin.[18] In closing, we note that one can combine Eqs. (74) and (75) to obtain a properly symmetrized form of the "Lagrangian."

APPENDIX C: HOT-ELECTRON GREEN'S FUNCTION

We take a simple Hamiltonian of free electrons subjected to a very intense electric field. This model is of some relevance to the formulation of high-field carrier transport in submicron devices;

$$\mathscr{H}=\int\hat{\psi}^\dagger(x)\left[\frac{-\hbar^2}{2m}\nabla^2-x\cdot F\right]\psi(x)dx , \tag{C1}$$

where F is the electric field. The one-particle Green's function is defined by

$$G(x,t,x',t')=\frac{1}{i\hbar}\langle T\psi(x,t)\psi^\dagger(x',t')\rangle . \tag{C2}$$

For hot-electron physics, we may take our ground state to

be the vacuum or empty band. The Heisenberg equation of motion is

$$\frac{i\hbar\partial\psi(x,t)}{\partial t}=e^{(i/\hbar)\mathscr{H}t}[\psi(x),\mathscr{H}]e^{-(i/\hbar)\mathscr{H}t}$$
$$=[\psi(x,t),\mathscr{H}]\ , \tag{C3}$$

so that the time dependence of the field operation is in general given by

$$\psi(x,t)=e^{(i/\hbar)\mathscr{H}t}\psi(x,0)e^{-(i/\hbar)\mathscr{H}t}\ . \tag{C4}$$

However, for the Hamiltonian of Eq. (C1), the right-hand side of Eq. (C3) is linear in the field operator and becomes

$$i\hbar\frac{\partial\psi(x,t)}{\partial t}=\left[\frac{-\hbar^2}{2m}\nabla^2-x\cdot F\right]\psi(x,t)=\tilde{\mathscr{H}}\psi(x,t)\ , \tag{C5}$$

where $\tilde{\mathscr{H}}$ is independent of the field operators. Therefore, we can also write the field dependence of $\psi(x,t)$ as

$$\psi(x,t)=e^{-(i/\hbar)\tilde{\mathscr{H}}t}\psi(x,0)\ . \tag{C6}$$

Equation (C2) for the Green's function can therefore be written as

$$G(x,t;x't')$$
$$=\frac{1}{i\hbar}\Theta(t-t')\langle 0\,|\,\psi(x,0)e^{-(i/\hbar)\tilde{\mathscr{H}}(t-t')}\psi^{\dagger}(x',0)\,|\,0\rangle$$
$$=\frac{1}{i\hbar}\Theta(t-t')\langle x\,|\,e^{-(i/\hbar)\tilde{\mathscr{H}}(t-t')}\,|\,x'\rangle\ , \tag{C7}$$

where ket and bra denotes the eigenvectors of position operator.[52] Therefore, we have reduced the problem to finding the kernel or propagator of a Schrödinger equation to a Feynman path integral with Hamiltonian $\tilde{\mathscr{H}}$. We can immediately write[13]

$$\langle x\,|\,e^{-(i/\hbar)\tilde{\mathscr{H}}(t-t')}\,|\,x'\rangle=\langle x\,|\,U(t,t')\,|\,x'\rangle$$
$$=\lim_{n\to\infty}\int\left[\prod_{i=1}^{n}d^3q_i\right](m/2\pi i\hbar\epsilon)^{3(n+1)/2}\exp\left[\frac{im}{2\hbar\epsilon}\sum_{i=1}^{n+1}(q_i-q_{i-1})^2+\frac{\epsilon^2}{m}\mathbf{F}\cdot(\mathbf{q}_i+\mathbf{q}_{i-1})\right]\ , \tag{C8}$$

where $q_{n+1}=x$ and $q_0=x'$. Equation (C8) represents a set of Gaussian integrals. The integration may be carried out on one variable after the other. In this manner, a recursion process[13] can be established, and after $3n$ integration we have in the limit $n\to\infty$

$$\langle x\,|\,U(t,t')\,|\,x'\rangle=\left[\frac{2\pi i\hbar(t-t')}{m}\right]^{-3/2}\exp\left[\frac{im}{2\hbar(t-t')}\left[|\,\mathbf{x}-\mathbf{x}'\,|^2+(t-t')^2\frac{\mathbf{F}\cdot(\mathbf{x}+\mathbf{x}')}{m}\right]\right]\exp\left[\frac{-im(t-t')^3}{24\hbar}\left|\frac{\mathbf{F}}{m}\right|^2\right], \tag{C9}$$

where $t-t'=(n+1)\epsilon$, $n\to\infty$, $\epsilon\to 0$. We now take the Fourier transform of Eq. (C7), using Eq. (C9),

$$G(k,k',t,t')=\frac{1}{(2\pi)^3}\int\int G(x,t;x't')e^{-ik\cdot x}e^{ik'\cdot x'}dx\,dx'\ .$$

By making a change of variables, $(x-x')=w$, and integrating over w and x' variables, where the integrals are all Gaussian, we obtain

$$G(k,k',t,t')=-\frac{i}{\hbar}\Theta(t-t')\delta(\mathbf{k}-[\mathbf{k}'+(\mathbf{F}/\hbar)(t-t')])\exp\left[-\frac{i}{\hbar}\int_0^{t-t'}\frac{|\,\hbar\mathbf{k}-\tau\mathbf{F}\,|^2}{2m}d\tau\right]\ . \tag{C10}$$

Equation (C10) was also obtained by Jauho and Wilkins,[53] in their discussion of nonlinear transport properties, by solving the equation for the Green's function. The virtue of the calculation presented here is that path-integral formulation allows for a generalization to a wider class of problems.

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