

Analytical solution for the Fermi-sea energy of two-dimensional electrons in a magnetic field: Lattice path-integral approach and quantum interference

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We derive an exact solution for the total kinetic energy of noninteracting spinless electrons at half-filling in two-dimensional bipartite lattices. We employ a conceptually different approach that maps this problem exactly into a Feynman-Vdovichenko lattice walker. The problem is then reduced to the analytic study of the sum of magnetic phase factors on closed paths. We compare our results with the ones obtained through numerical calculations.

INTRODUCTION

Noninteracting tight-binding electron models at half-filling in two-dimensional (2D) bipartite (e.g., square and hexagonal) lattices have recently received renewed attention due to their role in condensed matter¹ and particle physics.² For instance, several quantum field theories² arise in a natural way from 2D tight-binding lattice fermion problems at half-filling for hexagonal^{1,2} (e.g., 2D graphite³) and square lattices.^{2,4} These quantum field theories² are important to the problem of dynamical symmetry breaking, which plays a central role in many current areas of research; for instance, they provide a possible mechanism for generating the fermion mass spectrum in elementary particle physics.⁵ Furthermore, noninteracting 2D tight-binding electrons in a perpendicular magnetic field have been the subject of intense study in areas of current interest like mesoscopic structures and the quantum Hall effect. More recently, the behavior of the kinetic energy of a 2D noninteracting electron gas under the influence of both a periodic potential and a magnetic field has been analyzed by Hasegawa *et al.*⁶ and many others.^{7,8} These results have been related to mean-field approaches to the t - J model⁸ of high-temperature superconductors. It is of value to obtain analytical results for this important problem that has recently motivated many perturbative and numerical studies.

The goal of this paper is to present exact results that relate the kinetic energy of the half-filled Fermi sea of tight-binding electrons with sum-over-paths on the lattice. The problem is then reduced to the study of phase factors on closed paths. From the computational point of view, we would like to present an alternative to the standard approaches. From a physical point of view, and following Feynman's program, we would like to reformulate this quantum problem as an "average over histories."

Recently, the lattice path approach has also been applied to two very diverse problems; the computation of (1) equilibrium crystal shapes,⁹ and (2) the superconducting transition temperature in wire micronetworks and Josephson-junction arrays.¹⁰

FERMI-SEA ENERGY

The kinetic energy of spinless electrons on a 2D lattice in a uniform magnetic field is described by the Hamiltonian $H = -\sum_{\langle ij \rangle} c_i^\dagger c_j \exp[i\phi_{ij}]$, where $\langle ij \rangle$ refers to nearest-neighbor sites and $\phi_{ij} = 2\pi \int_i^j \mathbf{A} \cdot d\mathbf{l}$ in units of the flux quantum. Also, $|j\rangle \equiv c_j^\dagger |0\rangle$ defines a localized state centered at site j , and we will work on the $\{|j\rangle\}$ basis. The above Hamiltonian has a fractal quantum energy spectrum as a function of an applied magnetic field and also plays a central role in the physics of particles with fractional statistics (anyons).¹¹

At half-filling, the Fermi-sea ground-state energy is the sum of the lowest $N/2$ eigenvalues, where N is the total number of sites. Since the energy spectra of bipartite (e.g., square and hexagonal) lattices are symmetric under $\{E\} \rightarrow \{-E\}$, we can write the Fermi-sea ground-state energy per site as $E_T = \frac{1}{N} \sum_{E < 0} E = -(z/2N) \text{Tr} |H_0/z|$. Here, H_0 is the corresponding diagonalized Hamiltonian obtained from H by a similarity transformation. Also z is the coordination number of the lattice and Tr denotes the trace. For a square (honeycomb) lattice, $z = 4$ (3). Note that the energy spectrum of a lattice is bounded between $-z$ and z . By expanding $|x| \equiv |H_0/z|$ into a Chebyshev series $T_{2k}(x)$, it follows that

$$|x| = \frac{2}{\pi} + \frac{4}{\pi} \sum_{k \geq 1} \frac{(-1)^{k+1}}{4k^2 - 1} T_{2k}(x).$$

Also, using the identity

$$T_{2k}(x) = (-1)^k k \sum_{l=0}^k (-1)^l \frac{(k+l-1)!}{(k-l)!(2l)!} (2x)^{2l},$$

we obtain

$$E_T = -\frac{z}{N\pi} \left[1 - 2 \sum_{k \geq 1} \frac{k}{4k^2 - 1} \left(\sum_{l=0}^k \Gamma_l \text{Tr}(H^{2l}) \right) \right], \quad (1)$$

where

$$\Gamma_l = \left(\frac{-4}{z^2}\right)^l \frac{(k+l-1)!}{(2l)!(k-l)!}.$$

We have replaced $\text{Tr}(H_0^{2l})$ by $\text{Tr}(H^{2l})$, as they are equal to each other.

Now let us examine the term $\text{Tr}(H^{2l})$ more closely. Assuming periodic boundary conditions on the lattices, we have

$$\begin{aligned} \text{Tr}(H^{2l}) &= \langle 1|H^{2l}|1\rangle + \langle 2|H^{2l}|2\rangle + \cdots + \langle N|H^{2l}|N\rangle \\ &= N\langle j|H^{2l}|j\rangle. \end{aligned} \quad (2)$$

The Fermi-sea ground-state energy is then exactly given by

$$E_T(\Phi) = -\frac{z}{\pi} \left[1 - 2 \sum_{k \geq 1} \frac{k}{4k^2 - 1} \left(\sum_{l=0}^k \Gamma_l M_{2l}(\Phi) \right) \right], \quad (3)$$

where Φ equals 2π times the flux through each lattice plaquette, and $M_{2l}(\Phi) \equiv \langle j|H^{2l}|j\rangle$ is a moment, or lattice path integral, discussed in more detail below.

We have also studied two additional expansion schemes; one of them using a different set of orthogonal polynomials and the other based on a power series. One of them exploits the expansion of $|x|$ in terms of Legendre polynomials, $P_{2k}(x)$, as

$$|x| = \frac{1}{2} + \sum_{k \geq 1} \frac{(2k-3)!!}{(2k+2)!!} (4k+1) P_{2k}(x).$$

After expressing each $P_{2k}(x)$ in terms of a power series, it is clear that

$$\begin{aligned} E_T(\Phi) &= -\frac{z}{4} \left[1 - 2 \sum_{k \geq 1} \frac{4k+1}{4^k} \frac{(2k-3)!!}{(2k+2)!!} \right. \\ &\quad \left. \times \left(\sum_{l=0}^k \Omega_l M_{2l}(\Phi) \right) \right], \end{aligned} \quad (4)$$

where

$$\Omega_l = \left(\frac{-1}{z^2}\right)^l \frac{(2k+2l)!}{(2l)!(k-l)!(k+l)!}.$$

The other scheme starts by rewriting E_T as follows:

$$\begin{aligned} E_T &= -\frac{1}{2N} \text{Tr}[(H_0^2)^{1/2}] \\ &= -\frac{a}{2N} \text{Tr} \left\{ \left[1 + \left(-1 + \frac{H_0^2}{a^2} \right) \right]^{1/2} \right\}, \end{aligned}$$

where a is a constant to ensure $|-1 + H_0^2/a^2| < 1$. In general, $a = 2\sqrt{2}$ for a square lattice, and $a = 3/\sqrt{2}$ for a honeycomb lattice. However, for a magnetic flux near $1/2$, we find that $a = 2$ produces better results for both lattice types, since the energy density vanishes for larger

values of $E = 2\sqrt{2}$. By direct series expansions, we then obtain

$$E_T(\Phi) = \frac{a}{2} \left[-1 + \sum_{k \geq 1} \Lambda_k \left(\sum_{l=0}^k \frac{(-1)^l k!}{(k-l)!!} \frac{1}{a^{2l}} M_{2l}(\Phi) \right) \right] \quad (5)$$

with

$$\Lambda_k = \frac{1}{2^{2k-1} k} \frac{(2k-2)!}{[(k-1)!]^2}.$$

Among the above three solutions for $E_T(\Phi)$ [namely, Eqs. (3)–(5)], Eq. (3) gives the best results because of its relatively rapid convergence. We will return to the discussion on their accuracy later.

SUM OVER PATHS

The lattice path integral (or moment) used in this work is

$$M_{2l} \equiv \langle j|H^{2l}|j\rangle = \sum_{\text{All 2D closed paths}} e^{i\Phi_c}, \quad (6)$$

where $\Phi_c/2\pi$ is equal to the net flux enclosed by the directed closed path and $2l$ is referred as its order. The physical meaning of the above quantum mechanical expectation value is simple. The Hamiltonian H is applied $2l$ times to the initial state $|j\rangle$ localized at site j . This provides enough kinetic energy for the electron to hop through $2l$ bonds, reaching the new state $H^{2l}|j\rangle$ located at the end of the path. The above expectation value is nonzero only when the path ends at the starting site j . In our problem, quantum interference arises because the phase factors of different closed paths, or separate contributions from the same path, interfere with each other, sometimes producing cancellations in the phases. Therefore, our calculations generalize the Aharonov-Bohm phase factor, obtained by having an electron going around a single flux-enclosing loop, to the (multiply connected) lattice case.

The basic problem is now reduced to the computation of the lattice path integrals. This is a very difficult task, since each moment involves an enormous number of different loops, each one weighted by its corresponding phase factor. We have considerably simplified this calculation by analyzing the symmetries of the problem. In the next few paragraphs, we will list the most important symmetries involved and we will present a few examples of how the method works. Further details, with applications of this method to other problems, will be presented elsewhere.

We will now compute M_{2l} . We consider a unit spacing for square as well as graphite lattices and employ the Landau gauge $\mathbf{A} = (0, Bx)$. Note that M_0 equals 1 and is independent of the type of lattice. Also, the M_{2l} 's

are gauge invariant. First let us investigate the square lattice. Writing the coordinates of site j as $j = (m, n)$, we define an auxiliary quantity, $W_r(m, n)$, which is the sum over all possible paths of r steps on which an electron may hop from some given site to the site (m, n) . From the definition of $W_r(m, n)$, it is evident that it obeys the recurrence relation

$$W_{r+1}(m, n) = W_r(m \pm 1, n) + e^{\mp im\Phi} W_r(m, n \pm 1). \quad (7)$$

Equation (7) states that the site (m, n) can be reached by taking the $(r + 1)$ th step from the four nearest-neighbor sites. The factors in front of the W_r 's account for the presence of the magnetic field. We can construct further recurrence relations successively. For example,

$$W_{r+2}(m, n) = 4W_r(m, n) + (1 + e^{\pm i\Phi})[e^{im\Phi} W_r(m \pm 1, n - 1) + e^{-im\Phi} W_r(m \mp 1, n + 1)] + W_r(m \pm 2, n) + e^{\pm 2im\Phi} W_r(m, n \mp 2). \quad (8)$$

Examining the action of the Hamiltonian on the state $|j\rangle = |m, n\rangle$, we find that

$$-H|m, n\rangle = |m \pm 1, n\rangle + e^{\mp im\Phi} |m, n \pm 1\rangle. \quad (9)$$

Hence, by comparing Eq. (7) with Eq. (9), we obtain M_{2l} which is just the coefficient of $W_r(m, n)$ in the recurrence relation for $W_{r+2l}(m, n)$. This coefficient is obviously *the sum over all possible paths* which return an electron to its original site (m, n) after hopping $2l$ steps. Each path has a phase factor corresponding to the net flux going through the *directed* (e.g., $-\Phi_c$ clockwise and Φ_c counterclockwise) path.

It is worthwhile to notice the following symmetries when constructing recurrence relations and obtaining M_{2l} .

(a) The recurrence relation for W_{r+l} contains only terms $W_r(m + p, n \pm q)$ and $W_r(m - p, n \pm q)$ which satisfy the restriction $p + q = 1, 3, \dots, l$, for l odd and $= 0, 2, \dots, l$, for l even.

(b) The coefficients in front of the W_r 's can be factored into two parts. Each multiplicative factor involving coordinate m is always of the form $e^{\mp iqm\Phi}$, for $W_r(m + p, n \pm q)$ and $W_r(m - p, n \pm q)$. We shall refer to the rest of the prefactors (the part not involving m) as C_r . For instance, $C_r(m \pm 1, n - 1) = C_r(m \mp 1, n + 1) = 1 + e^{\pm i\Phi}$ in the above expression [Eq. (8)] for $W_{r+2}(m, n)$. These C_r 's satisfy $C_r(m + p, n - q) = C_r(m - p, n + q) = C_r(m + q, n - p) = C_r(m - q, n + p)$ and $C_r(m + p, n + q) = C_r(m - p, n - q) = C_r(m + q, n + p) = C_r(m - q, n - p)$. It can be shown that the latter set becomes equivalent to the former one when $\Phi \rightarrow -\Phi$ (and vice versa).

(c) To obtain M_{2l} , it is sufficient to compute the complete recurrence relation for $W_{r+l}(m, n)$.

We have computed the path integrals up to M_{40} . Here we list M_2 through M_{10} : 4, $28 + 8 \cos \Phi$, $232 + 144 \cos \Phi + 24 \cos 2\Phi$, $2156 + 2016 \cos \Phi + 616 \cos 2\Phi + 96 \cos 3\Phi + 16 \cos 4\Phi$, $21\,944 + 26\,320 \cos \Phi + 11\,080 \cos 2\Phi + 3120 \cos 3\Phi + 840 \cos 4\Phi + 160 \cos 5\Phi + 40 \cos 6\Phi$, for $l = 2, \dots, 10$. Notice that moments with odd orders are always zero because there is no path with an odd number of hops for which the electron may return to the initial site on a bipartite lattice.

We now consider the hexagonal lattice, which consists of two interpenetrating triangular sublattices. Following similar techniques, we have two different formulas for

$W_{r+1}(m, n)$. The proper choice between them depends on the sublattice to which the site (m, n) belongs. However, both choices lead to the same results for the path integrals. These have been computed up to M_{60} . We list M_2 through M_{10} here: 3, 15, $87 + 6 \cos \Phi$, $543 + 96 \cos \Phi$, $3543 + 1080 \cos \Phi + 30 \cos 2\Phi$, for $l = 2, \dots, 10$.

In general, the path integrals can be analytically computed by hand to any desired order through the techniques discussed above. We have computed by hand the moments up to the 20th order for both square and hexagonal lattices. However, these and the higher-order moments can be most conveniently obtained by using computer symbolic-manipulation software. The correctness of the calculated moments is assured by the consistency of the results obtained by hand and by computer.

FERMI-SEA ENERGY VALUES AND DISCUSSION

After computing the lattice path integrals, we can now proceed to calculate the kinetic energy of the half-filled Fermi sea. Recall that we have obtained the moments up to M_{40} (M_{60}) for the square (honeycomb) lattice. Therefore, by truncating the series at $k = 20$ (30) for a square (honeycomb) lattice in Eqs. (3)–(5), we obtain analytic closed-form expressions for the ground-state energy as an explicit function of the magnetic flux. In Table I, we present our results for the Fermi sea energies at various values of the flux by using Eqs. (3) and (4). For the square (hexagonal) lattice, the results are obtained by using the path integrals up to M_{20} , M_{30} , and M_{40} (M_{20} , M_{40} , and M_{60}), respectively. Here, instead of showing the exact numerical expressions (involving, e.g., π 's and square roots of integers), we present the actual numerical values for easier comparison purposes. It is worthwhile to notice that results obtained by using moments up to M_{20} are already in excellent agreement with those obtained in Refs. 6 and 7. The values obtained by using higher-order moments are essentially identical. Also Eq. (3) and Eq. (4) produce almost identical results. Although the results obtained from Eq. (5) are not as close as those obtained from Eqs. (3) and (4), they are consistent within ± 0.03 .

It should be pointed out here that the tight-binding

TABLE I. Fermi-sea ground-state energies at half-filling for the square and hexagonal lattices and for various values of the flux. The first three (fourth to sixth) rows present results obtained from Eq. (3) [Eq. (4)], i.e., by using a Chebyshev (Legendre) series expansion. The numbers in parentheses indicate the highest order of the path integral used. They are compared with the numerical results (Num.) from Refs. 6 and 7.

Square lattice							
$\frac{\Phi}{2\pi}$	0	1/8	1/6	1/4	1/3	3/8	1/2
C (20)	-0.8114920	-0.8254256	-0.8288598	-0.8592316	-0.8569940	-0.8801229	-0.9583405
C (30)	-0.8109902	-0.8231301	-0.8347727	-0.8599869	-0.8576158	-0.8775567	-0.9581710
C (40)	-0.8108108	-0.8252121	-0.8361273	-0.8588387	-0.8574827	-0.8774209	-0.9580550
L (20)	-0.8114462	-0.8250180	-0.8286112	-0.8603026	-0.8567193	-0.8799075	-0.9584124
L (30)	-0.8109779	-0.8234147	-0.8348405	-0.8600546	-0.8576395	-0.8777049	-0.9582486
L (40)	-0.8108047	-0.8254116	-0.8362933	-0.8587258	-0.8575003	-0.8774703	-0.9580659
Num.	-0.811	-0.826	-0.835	-0.859	-0.857	-0.880	-0.958
Hexagonal lattice							
$\frac{\Phi}{2\pi}$	0	1/4	1/3	1/2			
C (20)	-0.7869927	-0.7506642	-0.7489389	-0.7527022			
C (40)	-0.7872330	-0.7527290	-0.7506511	-0.7538837			
C (60)	-0.7872775	-0.7530423	-0.7509664	-0.7537718			
L (20)	-0.7869492	-0.7512373	-0.7486450	-0.7524125			
L (40)	-0.7872308	-0.7527266	-0.7506855	-0.7537969			
L (60)	-0.7872783	-0.7530359	-0.7510000	-0.7537457			
Num.	-0.787	-0.753	-0.751	-0.754			

model H does not include the diamagnetic energy of the tight-binding orbitals and the reduction of the hopping amplitude by the magnetic field. This issue is outside the scope of this paper. The interested reader can find a very detailed analysis of these points in Ref. 12 and references therein. We also note that an expression for the density of states, in terms of elliptic integrals and obtained through a completely different approach, has been known for some time and used, for instance, in Ref. 7. Also, several groups,^{6,7} including ours, have obtained results by other methods, including purely numerical approaches. Furthermore, different approaches on similar problems have been recently explored.¹³

In conclusion, the theory of electronic diamagnetism in two-dimensional lattices has been studied extensively due to its many applications in very diverse areas of physics. In particular, several computations of the Fermi-sea energy have recently attracted considerable atten-

tion by many workers. We use a conceptually novel approach that maps the problem exactly onto a Feynman-Vdovichenko lattice walker. More specifically, we derive an expression for the Fermi-sea kinetic energy at half-filling, as a function of a uniform perpendicular magnetic field, in terms of the quantum interference originating from the sum over 2D lattice closed paths, each loop weighted by the phase factor corresponding to the net flux enclosed. The energies obtained are essentially identical to the ones obtained through numerical calculations. We have shown that lattice path-integral techniques can be successfully applied to this system and we expect this approach to be applicable to many other electronic problems.

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³ The 2D hexagonal (graphite or honeycomb) lattice describes the atomic arrangement of carbon atoms in graphite, a highly anisotropic semimetal with a stacking structure of almost independent hexagonal layers, each one with one valence electron per site. Given the double spin degeneracy this means a half-filled band. The electron dynamics is then modeled by a tight-binding model. In this work, we will concentrate on the half-filled band case; thus, the ground state has positive energy states empty, and neg-

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