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Influence of the electron-electron interaction on electronic spectra and persistent currents in one-dimensional loops

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We consider N electrons in a one-dimensional loop enclosing a static magnetic flux. The electronic positions are described in terms of collective and relative coordinates. The corresponding partition of the Hilbert space is particularly convenient to investigate the electronic spectrum in the range of large electron-electron interaction. The electronic current is determined by the collective motion of the electrons. Thus, in absence of backscattering by a one-particle potential, the electron-electron interaction does not affect the persistent current associated with the electronic ground state. This is different when backscattering is present, since then collective and relative motions are coupled. We present a detailed study of the interplay between potential backscattering and electron-electron interaction, which is revealed by the resulting ground-state currents as well as by the electronic excitation spectra.

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I. INTRODUCTION

The rapid progress in nanodevice technology has raised a large interest in effects revealing the coherence of electronic states in mesoscopic systems. The case of small metallic rings is of particular interest in this context. Already two decades ago, Büttiker, Imry, and Landauer[1] predicted that, even in presence of elastic backscattering by a spatially varying one-particle potential, the electronic ground state of an isolated conducting ring enclosing a magnetic flux Φ will carry a current, which depends periodically on the magnetic flux with period $\Phi_0 = h/e$. Somewhat later, it was shown that these persistent currents will survive moderate inelastic scattering.[2–4] The existence of persistent currents associated with the electronic ground state has been confirmed experimentally by several groups.[5–13] Ref. 9 gives a recent review of the experimental and theoretical situation. The comparison of the experimental results with the theoretical predictions of Ref. 1 based on the one-electron approach shows that some experimental features cannot be described within that picture.

Persistent currents with the expected Φ_0 periodicity have been observed by Chandrasekhar *et al.*[6] and by Mailly *et al.*[7] in single Au and GaAs-AlGaAs loops. Similar oscillations with period Φ_0 are found for the magnetoresistance of small single Au, Al, and Ag loops.[8] Studying the magnetic response of an ensemble of 10^7 copper rings, Lévy *et al.*[5] found oscillations with period $\Phi_0/2$ rather than Φ_0. Analogous results have been obtained most recently for an ensemble of mesoscopic 10^5 Ag rings[12] as well as for 10^5 GaAs rings in AlGaAs.[13] The appearance of $\Phi_0/2$ periods can be attributed to ensemble averaging.[3,4,14] This explanation is corroborated by the results for ensembles containing only a small number of rings, where both Φ_0 as well as $\Phi_0/2$ oscillations are found.[10,11]

Experimentally, the sign of the $\Phi_0/2$ oscillations for the ensemble-averaged persistent currents in the vicinity of zero magnetic field corresponds to diamagnetic response. The theoretical prediction of the sign turns out to be rather difficult, since it requires the knowledge of the spin configuration in the electronic ground state (see eg. Refs. 15–17).

Another intriguing problem is the amplitude of the persistent currents. The currents observed in metallic loops are by two to three orders of magnitude larger than those expected from the one-electron theory.[5,6,10,12] This discrepancy has given rise to intense discussion. Apparently, the one-electron approach overestimates the electron backscattering by impurities. Quite interestingly, such a discrepancy is not found for semiconductor rings.[7,11,13]

It is quite obvious that Coulomb interactions should be taken into account over the small dimensions of the loops. Screening of the Coulomb part of the impurity potentials leading to reduced electron backscattering is expected to be most effective in metals.[18] More specifically, the e-e interaction has been invoked to explain the large persistent currents in metallic loops.[15–17,19–23] Another explanation has been attempted in Refs. 9,24,25, where the dc magnetic response of disordered ring systems is related with the dephasing by internal or external nonthermal equilibrium noise. Here again, e-e interactions are essential, since they determine the coupling of the electronic system to the fluctuating electromagnetic field.[24] The influence of zero-point fluctuations on the electronic ground state of a mesoscopic normal metal ring has been studied by Cedraschi *et al.*,[26] who found that the persistent currents at zero temperature are always suppressed by such a coupling.

In the present paper we investigate the N-electron states in one-dimensional loop systems for an arbitrary number of interacting electrons and for arbitrary one-particle potentials. We use the continuous real-space representation. This is different from the usually employed Hubbard models based on a discrete local representation. Our present approach has the advantage that cutoff problems due to a limited range of the one-electron energy spectrum are avoided. We restrict our discussion to the case of spinless electrons, the arguments remaining essentially the same when the spin is included. A description of the general system properties is given in Sec. II. In Sec. III we develop the basic ideas for the case of N

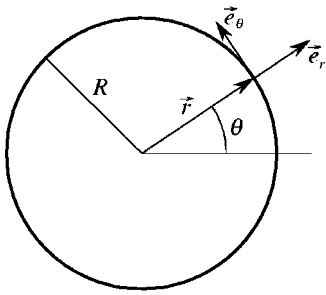

FIG. 1. Geometrical description of the sample system.

$=2$ electrons. Our approach, which is essentially based on the separation of collective and relative motion of the electrons, is then generalized in Sec. IV to VI to arbitrary N. In Sec. V we show that strong e-e interactions can be described very efficiently within a harmonic approximation. For constant one-particle potentials, collective and relative motions evolve independently of each other. Backscattering by a spatially varying one-particle potential leads to coupling between both types of motion. The resulting interplay between e-e interaction and potential backscattering is investigated in Sec. VI, where we discuss the persistent currents associated with the electronic ground state as well as the low-energy spectrum. The knowledge of the spectral properties is crucial to get an access to the dynamical response of loop structures to time-dependent external fields. Conclusions are drawn in Sec. VII.

II. THEORETICAL DESCRIPTION OF *N* ELECTRONS IN A LOOP

We consider N interacting spinless electrons in a circular one-dimensional loop of radius R (see Fig. 1). For convenience, we use polar coordinates in the following. External magnetic and electric fields $\vec{B}$ and $\vec{E}$ are represented by the vector potentials $\vec{A}(r,\theta,z)$ and the scalar one-particle potentials $V(r,\theta,z)$,

$$\vec{B}=\nabla\times\vec{A},\qquad \vec{E}=-\nabla V.$$

The electronic positions are determined by the angles $\theta_n \in\mathbb{R}$, $n=1,\ldots,N$. The electrons being confined to the loop, it is judicious to choose a gauge, where the tangential vector potential becomes independent of the angle, i.e.,

$$\vec{A}=A(\theta)\vec{e}_\theta=A\vec{e}_\theta .$$

The one-particle potential on the loop is given by $V(\theta)$.

In order to keep the arguments as simple as possible, we consider the spin part of the wave function to be symmetric, i.e., we will disregard the electron spins. The system being periodic in the angles θ_n, the appropriate Hilbert space then is

$$\mathcal{H}=\mathcal{P}(L_2([0,2\pi[^N)),$$

where $\mathcal{P}$ is the projector on the subspace of the antisymmetric functions. The electronic eigenstates of the system may be described by periodic functions Ψ defined over $\mathbb{R}^N$,

$$\Psi(\ldots,\theta_n+\lambda_n 2\pi,\ldots)=\Psi(\ldots,\theta_n,\ldots),$$
$$\lambda_n\in\mathbb{Z},\quad n=1,\ldots,N, \tag{1}$$

thus satisfying the periodic boundary conditions. The spatial wave function has to be antisymmetric with respect to the permutation of two particles,

$$\Psi(\ldots,\theta_k,\ldots,\theta_l,\ldots)=-\Psi(\ldots,\theta_l,\ldots,\theta_k,\ldots),$$
$$k\neq l. \tag{2}$$

According to Eq. (1), this implies that

$$\Psi=0 \quad\text{if}\quad \theta_n=\theta_{n'}+\lambda_{nn'}2\pi,\quad n\neq n',\quad \lambda_{nn'}\in\mathbb{Z}. \tag{3}$$

The function satisfies the time-independent Schrödinger equation

$$E\Psi=H\Psi, \tag{4}$$

with the N-particle Hamiltonian

$$H=H_0+H_{ee}+H_{eV}. \tag{5}$$

The operator H_0 is the free-electron Hamiltonian, H_{ee} describes the Coulomb interaction and H_{eV} represents the one-particle potential term. In the following we use international units. Then H_0 is given by

$$H_0=\sum_{n=1}^{N}\frac{1}{2m}(p_n-eA)^2,$$

where m is the free-electron mass, e is the electronic charge, and

$$p_n=-i\frac{\hbar}{R}\partial_n$$

is the momentum operator, ∂_n standing for ∂_{θ_n}. The distance between two electrons being $d_{nn'}=2R|\sin[(\theta_n-\theta_n')/2]|$, the Coulomb-repulsion term reads

$$H_{ee}=\sum_{1\leqslant n<n'\leqslant N}\frac{1}{4\pi\varepsilon_0}\,\frac{e^2}{2R\left|\sin\dfrac{\theta_n-\theta_{n'}}{2}\right|}.$$

The one-particle potential $V(\theta)$ is periodic in θ. The constant term in the Fourier decomposition of $V(\theta)$ is physically unimportant and will be omitted in the following. We thus write

$$H_{eV}=\sum_{n=1}^{N}V(\theta_n)=\sum_{\nu>0}V_\nu\sum_{n=1}^{N}e^{i\nu\theta_n}+\text{c.c.}$$

In polar coordinates, the position operator for one electron on a circular loop with radius R is

$$\vec{r}=R\vec{e}_r .$$

The velocity operator is given by

$$\vec{j}=\frac{i}{\hbar}[H,\vec{r}]=\frac{1}{m}(p-eA)\vec{e}_\theta .$$

The trajectory being circular, it is more convenient to use the angular-momentum operator

$$\vec{L}=\vec{r}\times(p-eA)\vec{e}_\theta=R(p-eA)\vec{e}_y,$$

which is normal to the plane of the loop, since $\vec{e}_y=\vec{e}_r\times\vec{e}_\theta$. The total angular-momentum operator for N electrons is

$$L=\sum_{n=1}^{N} R(p_n-eA).$$

To avoid clumsy prefactors and to simplify the discussions, it is convenient to normalize energy and angular-momentum units. Measuring the magnetic flux Φ,

$$\Phi=\int \vec{B}^t d\vec{\sigma}=\int \vec{A}^t d\vec{l}=2\pi RA,$$

in units of the flux quantum

$$\Phi_0=\frac{2\pi\hbar}{e}=\frac{h}{e}=4.14\,10^{-15}\ \text{V s},$$

one gets the normalized magnetic flux

$$a_0=\frac{\Phi}{\Phi_0}.$$

Expressed in the units $\hbar^2/(2mR^2)$ for the energy, $2mR^2/\hbar$ for the time and $\hbar$ for the angular momentum, the Hamiltonian terms and the angular momentum operator read

$$H_0=\sum_{n=1}^{N}(-i\partial_n-a_0)^2, \tag{6}$$

$$H_{ee}=\sum_{1\leq n<n'\leq N}\frac{\eta^2}{\left|\sin\frac{\theta_n-\theta_{n'}}{2}\right|}, \tag{7}$$

$$H_{eV}=\sum_{\nu>0}v_\nu\sum_{n=1}^{N}e^{i\nu\theta_n}+\text{c.c.}, \tag{8}$$

$$L=\sum_{n=1}^{N}(-i\partial_n-a_0). \tag{9}$$

In this energy scale, the e-e interaction parameter η^2 is

$$\eta^2=\frac{e^2mR}{\hbar^2 4\pi\varepsilon_0},$$

and the νth Fourier component of the one-particle potential becomes

$$v_\nu=\frac{2mR^2}{\hbar^2}V_\nu.$$

Subtracting the Schrödinger equations corresponding to two different fluxes a_0 and a_0', we get the generalized continuity equation

$$(E-E')\bar{\Psi}\Psi'$$
$$=-\sum_{n=1}^{N}(-i\partial_{\theta_n}+a_0-a_0')\cdot\{[\overline{(-i\partial_{\theta_n}-a_0)\Psi}]\Psi'$$
$$+\bar{\Psi}[(-i\partial_{\theta_n}-a_0')\Psi')]\}.$$

Integration over the angles leads to

$$(E-E')\langle\Psi|\Psi'\rangle$$
$$=-(a_0-a_0')[\langle L(a_0)\Psi|\Psi'\rangle+\langle\Psi|L(a_0')\Psi'\rangle]. \tag{10}$$

For the same flux $a_0=a_0'$, the eigenvectors $|\Psi\rangle$ and $|\Psi'\rangle$ corresponding to different energies are orthogonal, since then

$$(E-E')\langle\Psi|\Psi'\rangle=0.$$

The eigenvalues of the Hamiltonian given by Eqs. (6)–(8) will be denoted as $E_b(a_0)$, where $b=1,2,\ldots,$ is the band index. For two eigenstates Ψ and Ψ' belonging to the same band E_b, $E=E_b(a_0)$, and $E'=E_b(a_0')$, one obtains after division of Eq. (10) by $(a_0-a_0')\langle\Psi|\Psi'\rangle$ in the limit $a_0'\rightarrow a_0$,

$$\langle L\rangle=-\frac{1}{2}\frac{\partial E}{\partial a_0},$$

i.e., the slope of the energy band $E_b(a_0)$ yields the expectation value of the angular momentum.

At zero temperature, the electronic system will relax into its ground state. One may then measure the associated magnetic moment, which is directly related with the so-called "persistent current."[5–7] In the following we will rather refer to the "persistent angular momentum" defined as $L_{\text{pers}}=\langle L\rangle_{\text{ground state}}$.

In Refs. 5,7, loop areas $S_1=0.12\ \mu\text{m}^2$ and $S_2=5.7\ \mu\text{m}^2$ have been investigated. For a typical sample area $S=1.2\ \mu\text{m}^2$, which corresponds to a ring radius $R=0.62\ \mu$m, the above units are 10^{-7} eV for the energy, 10^{-9} s for the time, and the e-e interaction parameter is $\eta^2=10^4$ This already indicates that the e-e interaction is rather strong and cannot be treated as a perturbation.

III. TWO INTERACTING ELECTRONS

In order to introduce the general idea underlying our approach, we first consider the case of two electrons. The Hilbert space is $\mathcal{H}=\mathcal{P}(L_2([0,2\pi[^2))$. The terms (6), (7), and (8) of the Hamiltonian (5) become

$$H_0=(-i\partial_1-a_0)^2+(-i\partial_2-a_0)^2,$$

$$H_{ee}=\eta^2 W,\quad W=\frac{1}{\left|\sin\frac{\theta_1-\theta_2}{2}\right|},$$

$$H_{eV}=\sum_{\nu>0}v_\nu(e^{i\nu\theta_1}+e^{i\nu\theta_2})+\text{c.c.},$$

and the angular-momentum operator (9) is now given by

$$L=(-i\partial_1-a_0)+(-i\partial_2-a_0).$$

The stationary solutions of the Schrödinger equation (4) are periodic

$$\Psi(\theta_1+2\pi,\theta_2)=\Psi(\theta_1,\theta_2+2\pi)=\Psi(\theta_1,\theta_2),$$

and antisymmetric with respect to the exchange of the electrons,

$$\Psi(\theta_2,\theta_1)=-\Psi(\theta_1,\theta_2).$$

This implies that the wave function is zero when $\theta_1=\theta_2+\lambda 2\pi$, i.e.,

$$\Psi(\theta,\theta+\lambda 2\pi)=0,\quad \lambda\in\mathbb{Z}.$$

The eigenstates of the free-electron Hamiltonian H_0 satisfy the Schrödinger equation

$$E^{(0)}\psi=H_0\psi.$$

The eigenfunctions form an orthonormal basis in $\mathcal{H}$. They are given by the Slater determinants

$$\psi_{mn}=\langle\theta_1,\theta_2|m,n\rangle=\frac{1}{\sqrt{2}}(e^{im\theta_1}e^{in\theta_2}-e^{in\theta_1}e^{im\theta_2}),$$

with $m>n\in\mathbb{Z}$. The corresponding energies and expectation values of the angular momentum are

$$E_{mn}^{(0)}=(m-a_0)^2+(n-a_0)^2,$$

$$\langle L\rangle_{m,n}=m-a_0+n-a_0=-\frac{1}{2}\partial_{a_0}E_{mn}^{(0)}.$$

This basis in $\mathcal{H}$ is appropriate for calculations when the e-e interaction and the one-particle potential term can be treated as perturbations. A solution of the stationary Schrödinger equation may be written as

$$|\Psi_{\alpha\beta}\rangle=\sum_{m'n'}|m',n'\rangle\Phi_{\alpha\beta}^{m'n'}$$

with $\Phi_{\alpha\beta}\in l^2\otimes l^2$. Expressed in this basis, the Schrödinger equation reads

$$\Phi E=[(M-a_0\mathbb{I})^2+(N-a_0\mathbb{I})^2+\eta^2W+V]\Phi,$$

with the matrix elements

$$M_{mn}^{m'n'}=\langle m,n|M|m',n'\rangle=m\,\delta_{mn}^{m'n'},$$

$$N_{mn}^{m'n'}=\langle m,n|N|m',n'\rangle=n\,\delta_{mn}^{m'n'},$$

$$W_{mn}^{m'n'}=\langle m,n|W|m',n'\rangle,$$

$$V_{mn}^{m'n'}=\langle m,n|H_{eV}|m',n'\rangle.$$

The energy bands for the two-electron case are given in Figs. 2–4 for the e-e interaction parameters $\eta^2=0,1,10^3$ and different one-particle potentials.

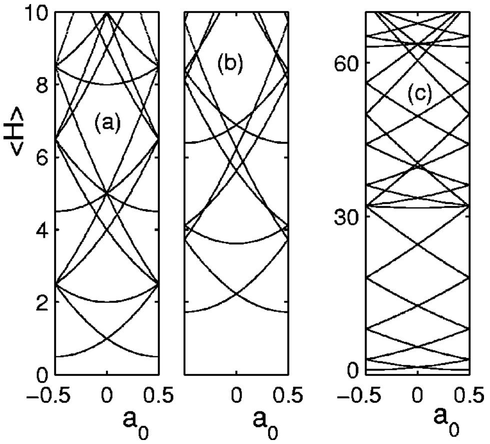

FIG. 2. Energy bands for two free electrons ($H_{eV}=0$) and for different e-e interaction parameters, (a) $\eta^2=0$, (b) $\eta^2=1$, and (c) $\eta^2=10^3$. There are no energy gaps. Note the different energy scale in (c).

To understand the effect of the e-e interaction, which depends only on the distance between the two electrons, it is convenient to introduce the collective and relative position coordinates u and c,

$$u=\frac{\theta_1+\theta_2}{2},\quad c=\frac{\theta_1-\theta_2}{2}. \tag{11}$$

The corresponding differential operators become

$$p_1=\frac{1}{2}(p_u+p_c),\quad p_2=\frac{1}{2}(p_u-p_c)$$

with $p_u=-i\partial_u$ and $p_c=-i\partial_c$. The total Hamiltonian may be written as

$$H=\frac{1}{2}(p_u-2a_0)^2+H_{\rm rel}+H_{eV}, \tag{12}$$

where

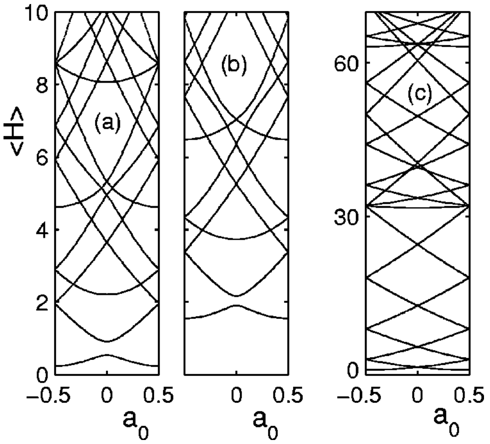

FIG. 3. Same as Fig. 2, but for included backscattering by a one-electron potential ($v_1=0.5$). The energy gaps due to potential backscattering decrease with increasing e-e interaction parameter η^2.

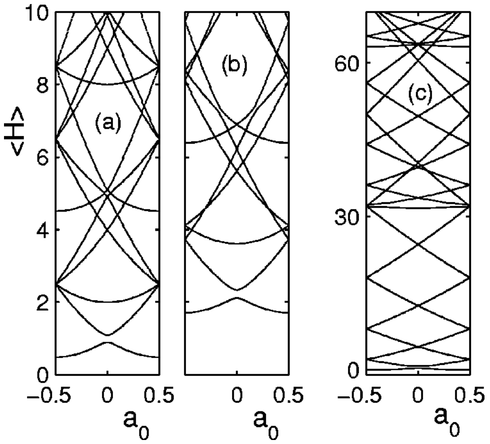

FIG. 4. Same as Fig. 2, but for included backscattering by a one-electron potential ($v_2=0.1$). The energy gaps due to potential backscattering slightly increase with increasing *e*-*e* interaction parameter η^2.

$$H_{\mathrm{rel}}=\frac{1}{2}p_c^2+\eta^2 W$$

determines the relative motion. The angular momentum operator

$$L=-i\partial_u-2a_0$$

acts only on the collective-motion coordinate. The *e*-*e* interaction, shown in Fig. 5(a), depends only on the relative distance,

$$W(c)=\frac{1}{|\sin c|}.$$

It thus has no effect on the persistent angular momentum as long as the collective and relative motions are uncoupled. In the ground state, the relative position approaches $c=\pi/2$ for increasing *e*-*e* interaction parameter η^2. In the limit of infinite interaction one gets

$$\lim_{\eta^2\to\infty} c=\frac{\pi}{2},$$

i.e., the distance between the electrons reaches its maximum value.

A one-particle potential term

$$H_{eV}=2\sum_{\nu>0}(v_\nu e^{i\nu u}+\overline{v}_\nu e^{-i\nu u})\cos(\nu c)$$

introduces backscattering. It leads always to a reduction of the persistent angular momentum $\langle L\rangle$. The reduction of $\langle L\rangle$ depends on the *e*-*e* interaction, since H_{eV} induces a coupling between the collective and the relative motions. To elucidate this dependence, we discuss the case of one-particle potentials with a single non-zero Fourier component.

The situation for $v_\nu=v_1\delta_{1\nu}$ is depicted in Fig. 5(b). It is seen that the *e*-*e* interaction confines the wave function in a region where the potential variations are small in the direction of the collective motion. The persistent angular momentum thus increases with the *e*-*e* coupling η^2. This case is representative for one-particle potentials described solely by nonzero Fourier components $v_{2\mu+1}$.

The case $v_\nu=v_2\delta_{2\nu}$ is presented in Fig. 5(c). In contrast with the above, the *e*-*e* interaction now confines the wave function in a region where the potential variations are large in direction of the collective motion. The resulting persistent angular momentum thus decreases with increasing *e*-*e* coupling η^2. This case is representative for one-particle potentials described solely by nonzero Fourier components $v_{2\mu}$.

The above analysis shows that the interaction between two electrons tends to suppress the backscattering due to the odd Fourier components $v_{2\mu+1}$ in H_{eV}. In the limit $\eta^2\to\infty$, only the even components $v_{2\mu}$ reduce the persistent angular momentum.

For small *e*-*e* interaction parameters η^2, the persistent angular momenta can easily be calculated using the basis of the Slater determinants of plane waves. For large *e*-*e* coupling, the number of basis vectors required to ensure a good accuracy increases rapidly. It is then preferable to use the collective and relative coordinates defined in Eq. (11).

For small one-particle potential terms H_{eV}, the eigenstates of the Hamiltonian H (12) for $H_{eV}=0$ provide a convenient basis of the Hilbert space $\mathcal{H}$. The symmetry properties of the wave functions can be easily expressed in the coordinates *u* and *c*. The spatial periodicity leads to

$$\Psi(u+\pi,c+\pi)=\Psi(u+\pi,c-\pi)=\Psi(u,c),$$

and the antisymmetry for the exchange of the electrons requires

$$\Psi(u,-c)=-\Psi(u,c).$$

In particular, we have

$$\Psi(u,\lambda\pi)=0,\quad \lambda\in\mathbb{Z},$$

and thus we may introduce separate cells *C* for the relative motion. With the choice

$$c\in C=[0,\pi[,$$

the spatial periodicity and the antisymmetry of the wave functions lead to the symmetry property

$$\Psi(u+\pi,\pi-c)=-\Psi(u,c). \tag{13}$$

The Hilbert space is

$$\mathcal{H}=\mathcal{P}(L_2([0,2\pi[\times[0,\pi[))$$

with the scalar product

$$\langle f|g\rangle=\frac{1}{2\pi}\int_0^{2\pi}du\frac{2}{\pi}\int_0^{\pi}dc\overline{f}(u,c)g(u,c).$$

In particular, the eigenstates of the Hamiltonian (12) for free and noninteracting electrons ($\eta^2=0$ and $H_{eV}=0$) are

$$\psi_{kn}(u,c)=e^{iku}\sin(nc),\quad k,n\ \ \text{with same parity,}$$

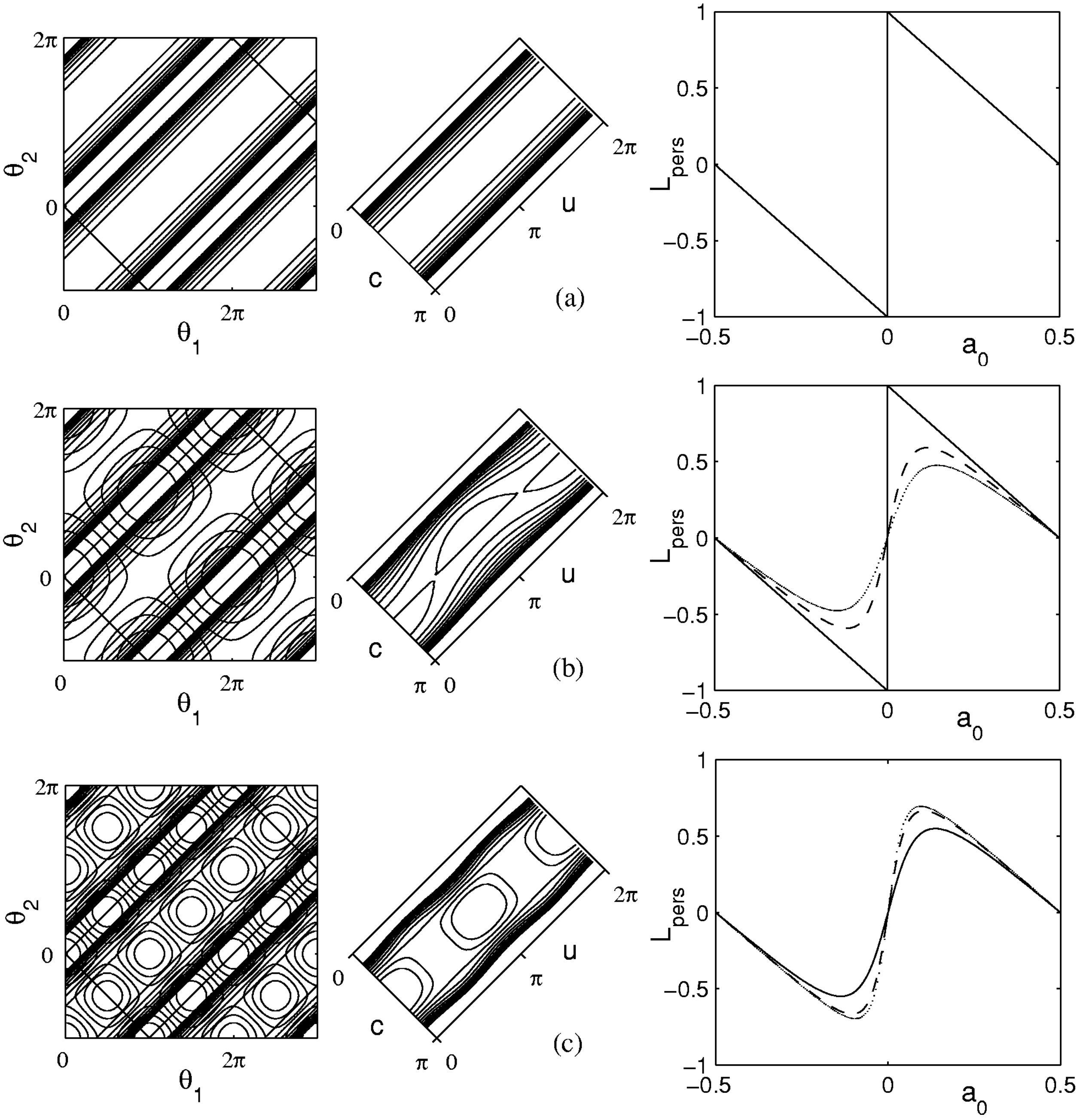

FIG. 5. One-particle potential term H_{eV} and e-e interaction potential H_{ee} (left and central column) for two electrons, and the corresponding persistent angular momenta (right column). The left column shows a schematic plot of the superimposed potentials H_{eV} and H_{ee} in the (θ_1,θ_2) plane for (a) $H_{eV}=0$, (b) $v_1\neq 0$, and (c) $v_2\neq 0$. The central column contains the summed potentials $H_{eV}+H_{ee}$. The corresponding persistent angular momenta are shown in the right column for (a) $H_{eV}=0$, (b) $v_1=0.5$, (c) $v_2=0.1$, and for the e-e interaction parameters $\eta^2=0$ (dotted line), $\eta^2=1$ (dashed line), and $\eta^2=10^3$ (full line). In absence of the one-particle potential term $H_{eV}=0$ [see (a)], the persistent angular momentum is independent of the e-e interaction parameter η^2. For $v_1\neq 0$ [see (b)], the persistent angular momentum rises with increasing η^2. For $v_2\neq 0$ [see (c)], the persistent angular momentum decreases with increasing η^2.

$$E_{kn}=\frac{1}{2}(k-2a_0)^2+\frac{1}{2}n^2,\quad k\in\mathbb{Z},\quad 1\leq n\in\mathbb{N}.$$

More generally, for interacting electrons ($\eta^2\neq 0$ and $H_{eV}=0$), one gets

$$\psi_{kn}(u,c)=e^{iku}\varphi_n(c),\quad k\in\mathbb{Z},\quad n\in\mathbb{N},$$

$$\mathcal{E}_n\varphi_n=H_{\mathrm{rel}}\varphi_n, \tag{14}$$

$$E_{kn}=\frac{1}{2}(k-2a_0)^2+\mathcal{E}_n,$$

where the indices k and n associated with the collective and the relative motion, respectively, are related through the symmetry property (13). Each mode n of the relative motion is associated with an infinite set of parabolic energy bands in $a_0 \in [-1/2,1/2[$ (Figs. 2–4). We note that the functions $\psi_{kn}(u,c)$ are the exact solutions including electronic correlation.

For large *e-e* coupling η^2, the lowest energy levels $\mathcal{E}_n$ for the relative motion may be calculated using the harmonic approximation of the *e-e* potential near its minimum in the cell C at $c=\pi/2$,

$$W(c)=\frac{1}{\sin c}\approx 1+\frac{1}{2}\left(c-\frac{\pi}{2}\right)^2.$$

The constant term is irrelevant and can be omitted. With the shift $q=c-\pi/2 \in Q=[-\pi/2,\pi/2[$, which corresponds to the choice of the origin at the center of the cell C, the relative motion is described by the Hamiltonian of the harmonic oscillator

$$H_{\mathrm{rel}}=\frac{1}{2}(-\partial_q^2+\eta^2 q^2).$$

Provided that the relevant eigenfunctions φ_n of the harmonic oscillator are sufficiently localized within the cell Q, one may replace the Hilbert space $\mathcal{H}=\mathcal{P}(L_2([0,2\pi[\times[-\pi/2,\pi/2[))$ by

$$\mathcal{H}=\mathcal{P}(L_2([0,2\pi[\times\mathbb{R}))$$

with the scalar product

$$\langle f|g\rangle=\frac{1}{2\pi}\int_0^{2\pi}du\int_{-\infty}^{\infty}dq\overline{f}(u,q)g(u,q).$$

Setting the ground-state energy to zero, the eigenvalues and eigenstates of H_{rel} are (see Appendix A)

$$\mathcal{E}_n=n\eta, \quad n\in\mathbb{N},$$

$$\varphi_n(q)=\frac{\eta^{1/4}}{\sqrt{2^n n!\sqrt{\pi}}}H_n(q\sqrt{\eta})e^{-q^2\eta^2/2}, \tag{15}$$

where $H_n(z)$ is the nth Hermite polynomial. For reasons of simplicity we use the same symbol φ in the above equation and for the function φ in Eq. (14), although both differ due to the shift of the origin. The high accuracy of the harmonic approximation is shown in Fig. 6, where we compare the exact energies $\mathcal{E}_n$ obtained by numerical solution of Eq. (14) with the corresponding values from the harmonic approximation.

With the new choice of the origin the symmetry property (13) becomes

$$\Psi(u+\pi,-q)=-\Psi(u,q).$$

A convenient basis of $\mathcal{H}$ is then provided by the eigenstates of H_0+H_{ee} in the harmonic approximation (15)

$$\psi_{kn}(u,q)=e^{iku}\varphi_n(q), \quad k,n \text{ with opposite parity}, \tag{16}$$

$$E_{kn}^{(0)}=\frac{1}{2}(k-2a_0)^2+n\eta, \quad k\in\mathbb{Z}, \quad n\in\mathbb{N}.$$

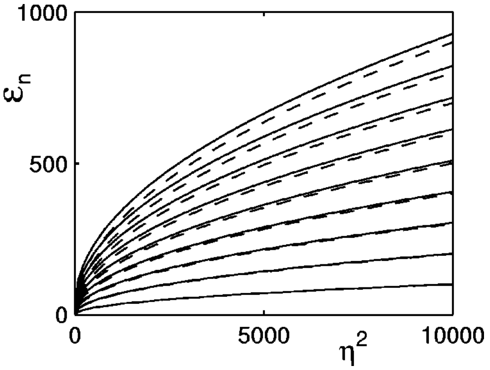

FIG. 6. Energies $\mathcal{E}_n$ associated with the relative motion as a function of the *e-e* interaction parameter η^2. Results obtained using the free-electron basis (solid lines); Results obtained in the harmonic approximation (dashed lines). The ground-state energy is set to zero.

The opposite parity of k and n follows from the symmetry of the Hermite polynomials.

With the coordinates u and c, the one-particle potential term reads

$$H_{eV}=2\sum_{\nu>0}(v_\nu e^{i\nu u}+\overline{v}_\nu e^{-i\nu u})\cos\left[\nu\left(q+\frac{\pi}{2}\right)\right].$$

Expressing the matrix elements $V_{kn}^{k'n'}$ of H_{eV} in the basis given by Eq. (16), we obtain the eigenstates of the Hamiltonian (12) from the solutions of the eigenvalue equation

$$\Phi E=[E^{(0)}+V]\Phi.$$

These solutions are exact for strong *e-e* interaction, since correlation effects are fully accounted for by the basis functions Eq. (16).

IV. *N* INTERACTING ELECTRONS

The normalized *e-e* interaction parameter η^2 being of the order of 10^4 for typical sample sizes (see Sec. II), we have to deal with strong electronic correlations. Thus, it is quite obvious that the basis formed by the eigenstates of the Hamiltonian for noninteracting electrons is not well suited to describe the influence of the *e-e* interaction on the eigenstates of the Hamiltonian (5). In the following we generalize the approach of the previous section introducing again collective and relative coordinates, but now for N electrons.

The N electron positions are described by the vector $\vec{\theta}\in\mathbb{R}^N$. The Hamiltonian given by Eqs. (6)–(8) acts in the Hilbert space $\mathcal{H}=\mathcal{P}(L_2([0,2\pi[^N))$. In analogy with the description of phonon modes in a one-dimensional ring of atoms, it is convenient to introduce the real cosine-Fourier transform of the coordinates. We define the N vectors $\vec{f}_n\in\mathbb{R}^{N-1}$, $n=1,\ldots,N$, by their $N-1$ components $j=1,\ldots,N-1$,

$$(\vec{f}_n)_j=\frac{\sqrt{2}}{\sqrt{N}}\cos\left(jn\beta_0+\frac{\pi}{4}\right), \quad \beta_0=\frac{2\pi}{N}.$$

These vectors are linearly dependent, since $\Sigma_{n=1}^{N}\vec{f}_n=\vec{0}$. The collective coordinate $u\in\mathbb{R}$ and the relative coordinates $\vec{c}\in\mathbb{R}^{N-1}$ are then expressed as

$$u=\frac{1}{N}\sum_n \theta_n, \quad \vec{c}=\sum_n \theta_n\vec{f}_n. \tag{17}$$

The position coordinates of the electrons can be written as (see Appendix B)

$$\theta_n=u+\vec{f}_n^t\vec{c}, \quad n=1,\dots,N. \tag{18}$$

Expressed in terms of the new coordinates u and $\vec{c}$, the Hamiltonian for free electrons reads (Appendix B)

$$H_0=\frac{1}{N}(-i\partial_u-Na_0)^2-\Delta_{N-1},$$

where $\Delta_{N-1}=\Sigma_{j=1}^{N-1}\partial_{c_j}^2$ is the Laplacian in $\mathbb{R}^{N-1}$. The e-e interaction term becomes

$$H_{ee}=\sum_{1\leqslant n<n'\leqslant N}\frac{\eta^2}{\left|\sin\left[\frac{1}{2}(\vec{f}_n^t-\vec{f}_{n'}^t)\vec{c}\right]\right|},$$

and the one-electron potential term is now given by

$$H_{eV}=\sum_{\nu>0}v_\nu e^{i\nu u}\sum_{n=1}^{N}e^{i\nu\vec{f}_n^t\vec{c}}+\text{c.c.}$$

The total angular momentum

$$L=-i\partial_u-Na_0 \tag{19}$$

depends only on the collective motion of the electrons.

The condition (3), which follows from the antisymmetry of the wave functions, now reads

$$\Psi=0 \quad \text{if} \quad \frac{1}{2}(\vec{f}_n^t-\vec{f}_{n'}^t)\vec{c}=\lambda_{nn'}\pi,\ n\neq n',\ \lambda_{nn'}\in\mathbb{Z}. \tag{20}$$

As expected, the collective coordinate u does not enter this condition.

The circular symmetry of the loop (1) as well as the antisymmetry condition (2) give rise to characteristic symmetry properties of the N-electron wave functions in $\mathbb{R}^N$. In the directions orthogonal to u, the antisymmetry imposes nodal planes of the wave functions. These planes, which are given by Eq. (20), delimit separate cells C in $\mathbb{R}^{N-1}$ (see examples in Appendix D). The space $\mathbb{R}^N$ is thus subdivided into identical prisms directed in the u direction, the cells C forming the bases. The function values in different cells being related by symmetry, it is sufficient to determine the wave functions within a single cell.

In the following we consider the particular cell C

$$0<\frac{1}{2}(\vec{f}_n^t-\vec{f}_{n'}^t)\vec{c}=\frac{1}{2}(\theta_n-\theta_{n'})<\pi,\quad 1\leqslant n<n'\leqslant N.$$

This choice corresponds to the specific ordering

$$\theta_1-2\pi<\theta_N<\cdots<\theta_2<\theta_1<\theta_N+2\pi. \tag{21}$$

Choosing the $N-1$ linearly independent vectors $\{\vec{f}_n\}_{n=1,\dots,N-1}$ as a basis of $\mathbb{R}^{N-1}$, one gets for a point $\vec{c}$ inside the cell (21)

$$\vec{c}=\sum_{n=1}^{N}(\theta_n-\theta_N)\vec{f}_n.$$

With $\sigma_i>0, i=1,\dots,N$ and $0<\sigma_{N-1}<\cdots<\sigma_1+\cdots+\sigma_{N-1}<\sigma_1+\cdots+\sigma_N=1$, we may also write

$$\theta_n-\theta_N=2\pi(\sigma_n+\cdots+\sigma_{N-1}),\quad n=1,\dots,N-1.$$

Thus, $\vec{c}$ is given by

$$\vec{c}=\sum_{i=1}^{N}\sigma_i\vec{S}_i \quad \text{with}\ \sigma_i>0 \ \text{and} \ \sum_{i=1}^{N}\sigma_i=1, \tag{22}$$

where

$$\vec{S}_1=2\pi\vec{f}_1,$$

$$\vec{S}_2=2\pi(\vec{f}_1+\vec{f}_2),$$

$$\vdots$$

$$\vec{S}_{N-1}=2\pi(\vec{f}_1+\cdots+\vec{f}_{N-1}),$$

$$\vec{S}_N=2\pi(\vec{f}_1+\cdots+\vec{f}_{N-1}+\vec{f}_N)=\vec{0},$$

are the summits of the cell $C\subset\mathbb{R}^{N-1}$ with the center

$$\vec{\Omega}=\frac{1}{N}\sum_{i=1}^{N}\vec{S}_i=\sum_{n=1}^{N}\Omega_n\vec{f}_n,\quad \Omega_n=\frac{2\pi}{N}(N-n).$$

Due to the circular symmetry of the loop, the wave functions must be periodic with respect to the translations $\theta_n\mapsto\theta_n+\lambda_n 2\pi$, $\lambda_n\in\mathbb{Z}$. Expressed in the new coordinates u and $\vec{c}$ defined in Eq. (17), these translations become

$$u\mapsto u+\lambda_n\frac{2\pi}{N},$$

$$\vec{c}\mapsto\vec{c}+\lambda_n 2\pi\vec{f}_n.$$

Accordingly, the periodicity condition (1) for the wave functions now reads

$$\Psi(u,\vec{c})=\Psi\left(u+\lambda_n\frac{2\pi}{N},\vec{c}+\lambda_n 2\pi\vec{f}_n\right),$$

$$\lambda_n\in\mathbb{Z},\quad n=1,\dots,N.$$

The exchange of two electrons corresponds to the commutation $(\theta_k,\theta_l)\mapsto(\theta_l,\theta_k), k\neq l$. Expressed in the coordinates u and $\vec{c}$, this operation is given by

$$u\mapsto u,$$

$$\vec{c}=\sum_{n=1}^{N}\theta_n\vec{f}_n\mapsto\sum_{n=1}^{N}\theta_n\vec{f}_n+(\theta_l-\theta_k)(\vec{f}_k-\vec{f}_l)$$

$$=\vec{c}-[(\vec{f}_k^t-\vec{f}_l^t)\vec{c}](\vec{f}_k-\vec{f}_l),$$

which follows directly from Eqs. (17) and (18). Since $\|\vec{f}_k-\vec{f}_l\|^2=2$ (see Appendix B), this corresponds to a reflection with respect to the hyperplane perpendicular to $\vec{f}_k-\vec{f}_l$, which is generated by the $N-2$ independent vectors $\vec{f}_n, n\neq k\neq l\neq n$. The antisymmetry condition (2) reads

$$\Psi(u,\vec{c})=-\Psi(u,\vec{c}-[(\vec{f}_k^t-\vec{f}_l^t)\vec{c}](\vec{f}_k-\vec{f}_l)),\quad k\neq l.$$

The conditions of periodicity and antisymmetry impose a symmetry property on the wave function inside the cell C. A permutation of two electrons θ_k and θ_l permutes $\vec{f}_k$ and $\vec{f}_l$ in Eq. (17). A cyclic permutation P_p of the electrons corresponds to the cyclic permutation

$$(\vec{f}_1,\ldots,\vec{f}_N)\mapsto(\vec{f}_{1+p},\ldots,\vec{f}_N,\vec{f}_1,\ldots,\vec{f}_p)$$

transforming $\vec{f}_n$ into $\vec{f}_{n+p}$. The indices are taken modulo N. A summit $\vec{S}_i$ of the cell C is thus transformed into $\vec{S}_{i+p}-\vec{S}_p$. The cell C is transformed into an identical cell, but translated by $-\vec{S}_p$ and with cyclically permuted summits. Accordingly, a point $\vec{c}^{(0)}\in C$ given by Eq. (22) transforms as

$$\vec{c}^{(0)}\mapsto\vec{c}_p^{(0)}=\sum_{i=1}^{N}\sigma_i\vec{S}_{i+p}-\vec{S}_p,$$

since $\Sigma_{i=1}^{N}\sigma_i=1$. Translating the cell back by $\vec{S}_p$, we obtain the initial cell but, due to the cyclic permutation of the summits, the resulting transformation of $\vec{c}^{(0)}$ is

$$\vec{c}^{(0)}\mapsto\vec{c}^{(p)}=\vec{c}_p^{(0)}+\vec{S}_p=\sum_{i=1}^{N}\sigma_i\vec{S}_{i+p},$$

with

$$\sigma_i>0,\ \sum_{i=1}^{N}\sigma_i=1.$$

As there are N cyclic permutations P_p, $p=1,\ldots,N$, this operation relates the wave functions at the N points $\vec{c}^{(p)}$ in the cell. A cyclic permutation P_p of N electrons can be decomposed into $p(N-1)$ permutations of two electrons. This leads to the multiplication of the wave function by $(-1)^{p(N-1)}$. While the permutations do not modify the collective position u, the translation $\vec{S}_p=2\pi(\vec{f}_1+\cdots+\vec{f}_p)$ leads to the transformation

$$u^{(0)}\mapsto u^{(p)}=u^{(0)}+p\frac{2\pi}{N}$$

because of the periodicity of the wave function in θ_n. For $p=1$, the conditions of periodicity and antisymmetry lead to

$$\Psi(u',\vec{c}')=(-1)^{N-1}\Psi(u,\vec{c}),\tag{23}$$

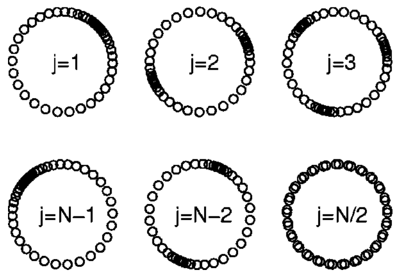

FIG. 7. Distortions of an electron lattice associated with different normal modes j for $N=50$ electrons.

with $u'=u+2\pi/N$, $\vec{c}=\vec{c}^{(0)}$, and $\vec{c}'=\vec{c}^{(1)}$. This defines the symmetry property of the wave function within the cell.

The result (23) can also be obtained directly from the cell definition (21). The cyclic permutation P_1 of the N electrons replaces electron $n-1$ by electron n, and the new position of electron n becomes θ_{n-1}. To restore the ordering of the electrons (21), one has then to move electron 1 to $\theta_N+2\pi$. Thus the new position θ_n' of electron n after these operations is

$$\theta_n'=\theta_{n-1}+2\pi\delta_{n1}.\tag{24}$$

With the new collective and relative coordinates u' and $\vec{c}'$ given by Eq. (17), we obtain again Eq. (23).

For convenience, we put the origin at the center $\vec{\Omega}$ of the cell C. The new relative position

$$\vec{q}=\vec{c}-\vec{\Omega}\in Q\subset\mathbb{R}^{N-1}\tag{25}$$

is a point in the shifted cell Q. In particular, the origin $\vec{q}=\vec{0}$ describes the configuration, where the N electrons are equally distributed on the ring. In this case the electrons form a lattice with the spacing $\beta_0=2\pi/N$. Using the relation

$$\vec{f}_n^t\vec{\Omega}=\vec{f}_n^t\sum_{j=1}^{N}\Omega_j\vec{f}_j=\frac{\pi}{N}(N+1-2n),$$

which follows directly from the properties of the vectors $\vec{f}_n$, we obtain for the position of electron n [Eq. (18)],

$$\theta_n=u+\frac{\pi}{N}(N+1-2n)+\frac{\sqrt{2}}{\sqrt{N}}\sum_{j=1}^{N-1}\cos\left(nj\beta_0+\frac{\pi}{4}\right)q_j.$$

The relative coordinate q_j defines the amplitude of a distortion j of the electron lattice. These distortions are illustrated for $N=50$ and $j=1,N-1,2,N-2,3,N/2$ in Fig. 7. The symmetry property (23) of the wave function becomes

$$\Psi(u',\vec{q}')=(-1)^{N-1}\Psi(u,\vec{q}).\tag{26}$$

Considering the pairs

$$q_j=\sum_n(\theta_n-\Omega_n)(\vec{f}_n)_j,\ q_{N-j}=\sum_n(\theta_n-\Omega_n)(\vec{f}_n)_{N-j}$$

for $j=1,\ldots,[(N-1)/2]$, and the identities

$$(\vec{f}_{n+1})_j=\frac{\sqrt{2}}{\sqrt{N}}\cos\left(j(n+1)\beta_0+\frac{\pi}{4}\right)$$

$$=\cos(j\beta_0)(\vec{f}_n)_j-\sin(j\beta_0)(\vec{f}_n)_{N-j},$$

$$(\vec{f}_{n+1})_{N-j}=\frac{\sqrt{2}}{\sqrt{N}}\cos\left(-j(n+1)\beta_0+\frac{\pi}{4}\right)$$

$$=\sin(j\beta_0)(\vec{f}_n)_j+\cos(j\beta_0)(\vec{f}_n)_{N-j},$$

we get under the transformation (24)

$$\begin{pmatrix} q'_j \\ q'_{N-j} \end{pmatrix}=\begin{pmatrix} \cos(j\beta_0) & -\sin(j\beta_0) \\ \sin(j\beta_0) & \cos(j\beta_0) \end{pmatrix}\begin{pmatrix} q_j \\ q_{N-j} \end{pmatrix}. \tag{27}$$

This describes a rotation with angle $j\beta_0$ in the (q_j, q_{N-j}) plane. For even N one has also

$$q_{N/2}=\frac{1}{\sqrt{N}}\sum_n(\theta_n-\Omega_n)(-1)^n$$

and

$$q'_{N/2}=-q_{N/2}.$$

The Hilbert space is

$$\mathcal{H}=\mathcal{P}(L_2([0,2\pi[\times Q)),$$

and the Hamiltonian terms are

$$H_0=\frac{1}{N}(-i\partial_u-Na_0)^2-\Delta_{N-1},$$

$$H_{ee}=\sum_{1\leqslant n<n'\leqslant N}\frac{\eta^2}{\left|\sin\left[\frac{1}{2}(\vec{f}^t_n-\vec{f}^t_{n'})(\vec{\Omega}+\vec{q})\right]\right|},$$

$$H_{eV}=\sum_{\nu>0}v_\nu e^{i\nu u}\sum_{n=1}^{N}e^{i\nu\vec{f}^t_n(\vec{\Omega}+\vec{q})}+\text{c.c.}, \tag{28}$$

where $\Delta_{N-1}=\Sigma_{j=1}^{N-1}\partial^2_{q_j}$ is the Laplacian in $\mathbb{R}^{N-1}$. The angular momentum L is given by Eq. (19).

V. ELECTRON-ELECTRON INTERACTION; HARMONIC APPROXIMATION

The e-e interaction potential $H_{ee}=\eta^2 W$ may be seen as a potential acting within the cell $Q\subset\mathbb{R}^{N-1}$. It is determined by the e-e interaction strength η^2 and

$$W=\sum_{1\leqslant n<n'\leqslant N}\frac{1}{\sin\left[\frac{1}{2}(\vec{f}^t_n-\vec{f}^t_{n'})(\vec{\Omega}+\vec{q})\right]}.$$

With the notation

$$a_{nn'}=\frac{1}{2}(\vec{f}^t_n-\vec{f}^t_{n'})\vec{\Omega}=\frac{\pi}{N}(n'-n)$$

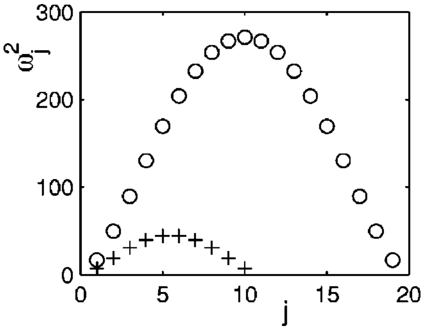

FIG. 8. Plasma frequencies ω_j for $N=11$ electrons (+) and for $N=20$ electrons (○).

and the second-order approximation

$$\frac{1}{\sin(a+h)}\approx\frac{1}{\sin a}-\frac{\cos a}{\sin^2 a}h+\frac{1+\cos^2 a}{2\sin^3 a}h^2,$$

we have

$$W\approx W_0+W_1+W_2.$$

The constant term

$$W_0=\sum_{1\leqslant n<n'\leqslant N}\frac{1}{\sin a_{nn'}}$$

may be set to zero for an appropriate choice of the zero of energy. The first-order term

$$W_1=-\frac{1}{2}\sum_{1\leqslant n<n'\leqslant N}\frac{\cos a_{nn'}}{\sin^2 a_{nn'}}(\vec{f}^t_n-\vec{f}^t_{n'})\vec{q}=0$$

vanishes (Appendix C). A strong e-e interaction H_{ee} may therefore be approximated by a parabolic potential with its minimum on the center of the cell Q. The second-order term becomes (Appendix C)

$$W_2=\sum_{1\leqslant n<n'\leqslant N}\frac{1+\cos^2 a_{nn'}}{2\sin^3 a_{nn'}}\left(\frac{1}{2}(\vec{f}^t_n-\vec{f}^t_{n'})\vec{q}\right)^2$$

$$=\sum_{j=1}^{N-1}\omega_j^2 q_j^2,$$

which corresponds to a sum of harmonic potentials. The plasma frequencies ω_j are given by

$$\omega_j^2=\sum_{\nu=1}^{N-1}\frac{1+\cos^2\frac{\nu\pi}{N}}{4\sin^3\frac{\nu\pi}{N}}\sin^2\frac{j\nu\pi}{N},\quad j=1,\dots,N-1.$$

The frequencies $\omega_j=\omega_{N-j}$, $j=1,\dots,[(N-1)/2]$ are degenerate except for even N, where the frequency $\omega_{N/2}$ is nondegenerate. Figure 8 shows the vibration frequencies for $N=11$ and $N=20$. The lowest plasma frequency may be approximated for large N (Appendix C) by

$$\omega_1^2=\omega_{N-1}^2\approx\frac{N}{\pi}\ln\frac{4N}{\pi\sqrt{\exp(1)}}.$$

The comparison with the numerical results shows that for $N>500$ this approximation differs by less than two percent from the exact result. The case of two electrons has already been discussed in Sec. III. The present general approach is illustrated in Appendix D for two, three, and four electrons.

With the harmonic approximation for the e-e interaction, it becomes possible to study the dynamics of an arbitrary number N of electrons in a static magnetic field. For sufficiently small one-particle potentials, a convenient basis of the Hilbert space

$$\mathcal{H}=\mathcal{P}(L_2([0,2\pi[\times\mathbb{R}^{N-1}))$$

is given by the eigenstates of the Hamiltonian

$$H_0+H_{ee}=\frac{1}{N}(-i\partial_u-Na_0)^2+H_{\mathrm{rel}}.$$

The Hamiltonian of the relative motion

$$H_{\mathrm{rel}}=-\Delta_{N-1}+\sum_{j=1}^{N-1}\eta^2\omega_j^2q_j^2$$

describes $N-1$ independent harmonic oscillators. Since collective and relative motions are uncoupled, the Hamiltonian is separable, and its eigenstates can be written

$$\psi(u,\vec{q})=e^{iku}\varphi(\vec{q}),$$

where

$$H_{\mathrm{rel}}\varphi=\mathcal{E}\varphi. \tag{29}$$

With an appropriate choice of the energy origin, the eigenvalues $\mathcal{E}$ are

$$\mathcal{E}=\sum_{j=1}^{N-1}2\eta n_j\omega_j\,,\ n_j\in\mathbb{N}.$$

The eigenfunctions $\varphi(\vec{q})$ are given by the product of $N-1$ one-oscillator eigenfunctions. They satisfy the symmetry condition (26),

$$e^{ik(2\pi/N)}\varphi(\vec{q}\,')=(-1)^{N-1}\varphi(\vec{q}), \tag{30}$$

which relates the symmetry of $\varphi(\vec{q})$ describing the relative motion with that of the collective motion labeled by k. This relation will be derived in the following.

Due to the degeneracy $\omega_j=\omega_{N-j}$, the Hamiltonian H_{rel}, restricted to the plane (q_j,q_{N-j}), $j=1,\ldots,[(N-1)/2]$, describes an isotropic two-dimensional harmonic oscillator. This suggests to use polar coordinates

$$q_j=r_j\cos\beta_j\,,\quad q_{N-j}=r_j\sin\beta_j\,. \tag{31}$$

The symmetry operations (27) correspond to a rotation in this plane, so that

$$(r_j',\beta_j')=(r_j,\beta_j+j\beta_0),\ \ j=1,\ldots,[(N-1)/2], \tag{32}$$

$$q'_{N/2}=-q_{N/2}\ \text{ if }\ N\ \text{ is even.}$$

The ground state of the relative motion (29) is given by (see Appendix A)

$$\mathcal{E}_0=0,$$

$$\varphi_0(\vec{q})=[\varphi_0^{(N/2)}(q_{N/2})]^{p_N}\prod_{j=1}^{[(N-1)/2]}\varphi_{00}^{(j)}(r_j,\beta_j)$$

$$=\left[\left(\frac{\eta\omega_{N/2}}{\pi}\right)^{1/4}e^{-q_{N/2}^2\eta\omega_{N/2}/2}\right]^{p_N}\prod_{j=1}^{[(N-1)/2]}\left(\frac{\eta\omega_j}{\pi}\right)^{1/2}e^{-r_j^2\eta\omega_j/2},$$

where p_N denotes the parity of N,

$$p_N=\begin{cases}1 & \text{if } N \text{ is even,}\\ 0 & \text{if } N \text{ is odd.}\end{cases}$$

Clearly, the ground state of the relative motion is invariant under the symmetry operations (32),

$$\varphi_0(\vec{q}\,')=\varphi_0(\vec{q}).$$

Thus the possible k values are given by $e^{ik(2\pi/N)}=(-1)^{N-1}$, i.e.,

$$k_0=\begin{cases}\mu N & \text{if } N \text{ is odd}\\ \left(\mu+\dfrac{1}{2}\right)N & \text{if } N \text{ is even}\end{cases}\qquad \mu\in\mathbb{Z}.$$

A first single-oscillator excitation has the energy

$$\mathcal{E}_1^{(j)}=2\eta\omega_j=\mathcal{E}_1^{(N-j)}.$$

Due to the twofold degeneracy for $j=1,\ldots,[(N-1)/2]$, the eigenfunctions are (see Appendix A)

$$\varphi_1^{(j)}(\vec{q})=\sqrt{\eta\omega_j}e^{i\beta_j}r_j\varphi_0(\vec{q}),$$

$$\varphi_1^{(N-j)}(\vec{q})=\sqrt{\eta\omega_j}e^{-i\beta_j}r_j\varphi_0(\vec{q}).$$

For even N we have

$$\varphi_1^{(N/2)}(\vec{q})=\sqrt{\eta\omega_{N/2}}q_{N/2}\varphi_0(\vec{q}).$$

With the symmetry of the wave function (30) and the transformation (32), the k values are given by $e^{ik(2\pi/N)}e^{i(j2\pi/N)}=(-1)^{N-1}$, $j=1,\ldots,N-1$, i.e.,

$$k_j=\begin{cases}\mu N-j & \text{if } N \text{ is odd}\\ \left(\mu+\dfrac{1}{2}\right)N-j & \text{if } N \text{ is even}\end{cases}\qquad \mu\in\mathbb{Z}.$$

More generally, the excited relative modes have the energies

$$\mathcal{E}=2\eta\omega_{N/2}n_{N/2}p_N+\sum_{j=1}^{[(N-1)/2]}2\eta\omega_j(2m_j+|l_j|)$$

and the eigenfunctions are

$$\varphi(\vec{q})=[\varphi n_{N/2}(q_{N/2})]^{p_N}\prod_{j=1}^{[(N-1)/2]}\frac{1}{\sqrt{2\pi}}e^{il_j\beta_j}R_{m_jl_j}(r_j).$$

According to the symmetry property (30) and the transformation (32), the admissible values for k are given by

$$k+\sum_{j=1}^{[(N-1)/2]}jl_j+\frac{N}{2}n_{N/2}p_N=\left(\mu+\frac{1}{2}p_N\right)N,\quad \mu\in\mathbb{Z}. \tag{33}$$

In the description of one-dimensional harmonic oscillators

$$m_j=\min(n_j,n_{N-j}),\qquad l_j=n_j-n_{N-j},$$

this becomes

$$k+\sum_{j=1}^{N-1}jn_j=\left(\mu+\frac{1}{2}p_N\right)N,\quad \mu\in\mathbb{Z}.$$

Resuming the indices describing a relative excitation by the index ϱ, the orthonormal basis $\{|k\varrho\rangle\}$ of $\mathcal{H}$ reads

$$\langle u,\vec{q}|k\varrho\rangle=e^{iku}\varphi_\varrho(\vec{q}),$$

$$E_{k\varrho}^{(0)}|k\varrho\rangle=(H_0+H_{ee})|k\varrho\rangle,$$

$$E_{k\varrho}^{(0)}=\frac{1}{N}(k-Na_0)^2+\mathcal{E}_\varrho. \tag{34}$$

VI. INFLUENCE OF THE ONE-PARTICLE POTENTIAL H_{eV}

In the basis developed in the previous section, the eigenstates of the total Hamiltonian including the one-particle potential term $H_{eV}\neq 0$ become

$$|\Psi\rangle=\sum_{k'\varrho'}|k'\varrho'\rangle\Phi_{k'\varrho'}.$$

They are the solutions of the Schrödinger equation

$$\Phi E=(E^{(0)}+V)\Phi,$$

with the matrix elements

$$E^{(0)}{}_{k\varrho}^{k'\varrho'}=E_{k\varrho}^{(0)}\delta_{k\varrho}^{k'\varrho'},$$

$$V_{k\varrho}^{k'\varrho'}=\langle k\varrho|H_{eV}|k'\varrho'\rangle.$$

The Fourier decomposition of the one-particle potential term (28) can be written as

$$H_{eV}=\sum_{\nu>0}v_\nu e^{i\nu u}I_\nu(\vec{q})+v_{-\nu}e^{-i\nu u}I_{-\nu}(\vec{q})$$

with $v_{-\nu}=\overline{v_\nu}$, and

$$I_\nu(\vec{q})=\sum_{n=1}^{N}\exp\left[i\nu\frac{\pi}{N}(N+1-2n)\right]\exp\left[i\nu\frac{\sqrt{2}}{\sqrt{N}}\sum_{j=1}^{N-1}r_j\sin\left(\beta_j+\frac{\pi}{4}-nj\beta_0\right)\right], \tag{35}$$

where the relative positions $\vec{q}$ are expressed in polar coordinates [see Eq. (31)]. Thus, the νth Fourier component of the matrix V is obtained from

$$V_{k\varrho}^{k'\varrho'}(\nu)=v_\nu\delta_k^{k'+\nu}\langle\varrho|I_\nu|\varrho'\rangle+v_{-\nu}\delta_k^{k'-\nu}\langle\varrho|I_{-\nu}|\varrho'\rangle.$$

The above expression shows that a component v_ν leads to a coupling between the collective states k and k' only when

$$|k-k'|=\nu. \tag{36}$$

In the following, our discussion will be restricted to odd electron numbers N, which implies that $p_N=0$. The extension to even N is straightforward, the difference between systems with N and $N+1$ electrons being essentially described by a shift $a_0\mapsto a_0+1/2$ for all physical quantities.[27]

The products

$$|\varrho\rangle=\otimes_{j=1}^{(N-1)/2}|m_jl_j\rangle=\otimes_{j=1}^{(N-1)/2}|ml\rangle_j,$$

which describe the eigenstates $|m_jl_j\rangle$, $m_j\in\mathbb{N}$, $l_j\in\mathbb{Z}$ of the $(N-1)/2$ two-dimensional harmonic oscillators (Appendix A), form a basis in the Hilbert space associated with the relative motion. The relative states, their energies and the possible values corresponding to the collective states k are given in Table I for the eight lowest energies of the relative motion. The symbols ○, ◁, ▷, and □ in the last column in Table I identify the minima of the energy bands for $N=11$ electrons shown in Fig. 9. Due to the degeneracy of the relative energies, minima at a_0 and $-a_0$ have the same energy.

The matrix elements $\langle\varrho|I_\nu|\varrho'\rangle$ (Appendix E) lead to a coupling between the relative states for

$$\nu+\sum_{j=1}^{(N-1)/2}(l_j-l_j')j=\mu N,\ \mu\in\mathbb{Z}.$$

This is consistent with the coupling condition (36) and the relation (33) between the collective and the relative states.

In presence of a weak one-particle potential, the ground state of the N-electron system is well described in the basis of the low-energy eigenstates of H_0+H_{ee}. According to condition (36), only Fourier components v_1, v_2, v_3, v_4, and v_N couple in first order between the first eight relative states (Appendix E). In the following, we choose a one-particle potential with nonzero components v_1 and v_N,

$$v_\nu=0,\quad \nu\neq 1,N.$$

With this restriction, the matrix elements of V are

$$V_{k\varrho}^{k'\varrho'}(1)=v_1\delta_k^{k'+1}\langle\varrho|I_1|\varrho'\rangle\ \ +v_{-1}\delta_k^{k'-1}\langle\varrho|I_{-1}|\varrho'\rangle, \tag{37}$$

TABLE I. Lowest excitation energies of the relative motion and corresponding k values. We use the notation $\overline{l}=-l$, and $|0\rangle_{j\geqslant 3}=\otimes_{j=3}^{(N-1)/2}|00\rangle_j$ denotes the ground state of the harmonic oscillators $j=3,\ldots,(N-1)/2$.

Excitation	Energy	State	Values for k	
Ground state	$\mathcal{E}_0=0$	$\lvert 0\rangle=\lvert 00\rangle_1\lvert 00\rangle_2\lvert 0\rangle_{j\geqslant 3}$	$k=\mu N$	(○)
First excitation	$\mathcal{E}_1^{(1)}=2\eta\omega_1$	$\lvert 1^{+1}\rangle=\lvert 01\rangle_1\lvert 00\rangle_2\lvert 0\rangle_{j\geqslant 3}$	$k+1=\mu N$	(◁)
		$\lvert 1^{-1}\rangle=\lvert 0\overline{1}\rangle_1\lvert 00\rangle_2\lvert 0\rangle_{j\geqslant 3}$	$k-1=\mu N$	(▷)
	$\mathcal{E}_1^{(2)}=2\eta\omega_2$	$\lvert 1^{+2}\rangle=\lvert 00\rangle_1\lvert 01\rangle_2\lvert 0\rangle_{j\geqslant 3}$	$k+2=\mu N$	(◁)
		$\lvert 1^{-2}\rangle=\lvert 00\rangle_1\lvert 0\overline{1}\rangle_2\lvert 0\rangle_{j\geqslant 3}$	$k-2=\mu N$	(▷)
Second excitation	$\mathcal{E}_2^{(1)}=4\eta\omega_1$	$\lvert 2^{+1}\rangle=\lvert 02\rangle_1\lvert 00\rangle_2\lvert 0\rangle_{j\geqslant 3}$	$k+2=\mu N$	(◁)
		$\lvert 2^{0}\rangle=\lvert 10\rangle_1\lvert 00\rangle_2\lvert 0\rangle_{j\geqslant 3}$	$k=\mu N$	(□)
		$\lvert 2^{-1}\rangle=\lvert 0\overline{2}\rangle_1\lvert 00\rangle_2\lvert 0\rangle_{j\geqslant 3}$	$k-2=\mu N$	(▷)

$$V_{k\varrho}^{k'\varrho'}(N)=v_N\delta_k^{k'+N}\langle\varrho|I_N|\varrho'\rangle+v_{-N}\delta_k^{k'-N}\langle\varrho|I_{-N}|\varrho'\rangle. \tag{38}$$

They are given in Appendix E.

The influence of the one-particle potential term H_{eV} and of the e-e interaction potential H_{ee} on the energy bands $\langle H\rangle(a_0)$ and on the persistent angular momentum $L_{\mathrm{pers}}(a_0)$ is shown in Figs. 10 and 11 for $N=1001$. In accordance with Table I, the energy bands for the same relative excitation $\mathcal{E}_\varrho$ are almost degenerate for large N.

The coupling induced by the one-electron potential term H_{eV} between two states decreases with their distance in energy. The strongest coupling occurs at the crossing of two energy bands (34) $E(a_0)=E'(a_0)$, which is situated at

$$a_0=\frac{k^2-k'^2+N\mathcal{E}_\varrho-N\mathcal{E}_{\varrho'}}{2N(k-k')},\quad |a_0|\leqslant\frac{1}{2}.$$

As can be seen in Fig. 10(a), such a band crossing does not occur for $|k-k'|=1$ in the considered energy region. This is due to the fact that excitation energies of the relative motion $\mathcal{E}_\varrho$ are rather large for the considered strong e-e interaction. The Fourier components v_1 thus only lead to a weak coupling. Band crossings are found for $|k-k'|=N$, where the Fourier components v_N then lead to a strong coupling. This is the case for $\mathcal{E}_\varrho=\mathcal{E}_{\varrho'}$ at the band edges $a_0=\pm\frac{1}{2}$. In particular, the ground state ($k=0$, $\mathcal{E}=0$) couples to the first bands ($k=\pm N$, $\mathcal{E}=0$). As seen in Fig. 10(b), a gap opens at the crossings. Correspondingly, the persistent angular momentum L_{pers} shown in Fig. 11 is reduced with respect to the angular momentum for $H_{eV}=0$. Following the same arguments, one finds again weak coupling for any Fourier components $v_\nu,\nu\neq N,2N,\ldots$. Only the Fourier components $v_{\mu N}$, $\mu\in\mathbb{N}$, give rise to a strong coupling.

In the limit of infinite e-e interaction ($\eta^2\to\infty$), all states with finite energies are associated with the ground state of the relative motion $|0\rangle$, i.e., the ground state of $N-1$ harmonic oscillators. The relative motion is completely localized at the center of the cell $\vec{q}=\vec{0}$ defined in Eq. (25). This corresponds to an even distribution of the N electrons on the circle,

$$\theta_n-\theta_{n+1}=\frac{2\pi}{N},\ n=1,\ldots,N-1.$$

According to Eq. (35), the contributions v_ν to the one-particle potential are suppressed for noninteger ν/N, as

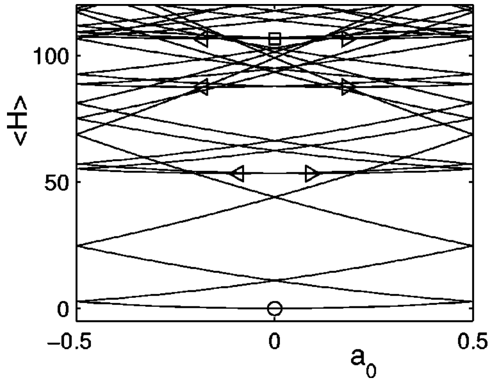

FIG. 9. Energy bands for $N=11$ interacting electrons in absence of a one-particle potential term ($H_{eV}=0$). The e-e interaction parameter is $\eta^2=10^2$. The symbols ○, ◁, ▷, and □ identify the minima of the bands corresponding to the states given in Table I.

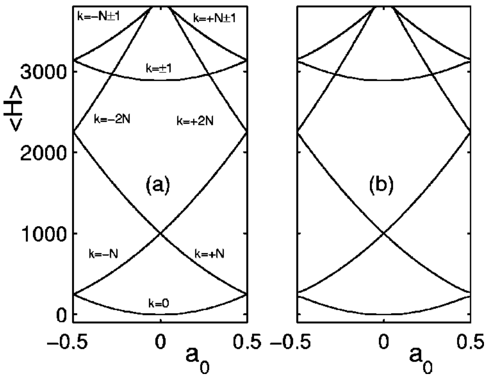

FIG. 10. Energy bands for $N=1001$ interacting electrons. The e-e interaction parameter is $\eta^2=10^3$. The results are given for (a) $H_{eV}=0$ and (b) $v_N=1$. The indicated k values identify the bands corresponding to the states given in Table I. For $v_N=1$, gaps are opened between energy bands k and k' when $k-k'=N$.

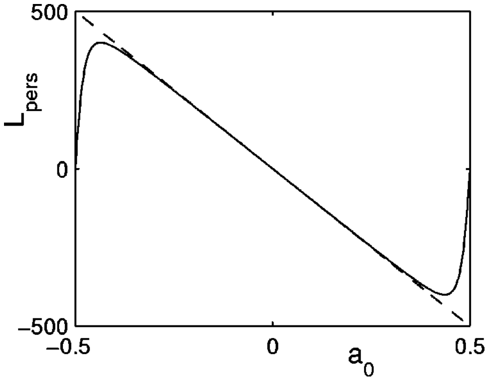

FIG. 11. Persistent angular momentum for $N=1001$ interacting electrons ($\eta^2=10^3$) for $H_{eV}=0$ (dashed line) and for $v_N=1$ (solid line).

$$\lim_{\eta^2\to\infty} \langle 0|I_\nu|0\rangle = I_\nu(\vec{0}) = \sum_{n=1}^{N} e^{i\nu(2\pi/N)n} = N\delta_\nu^{\mu N}, \quad \mu\in\mathbb{N}.$$

Only the Fourier-components $v_{\mu N}$, $\mu\in\mathbb{N}$, influence the collective position u and the angular momentum. This generalizes the result given for two electrons in Sec. III. In this limit, the N-electron system is described by the one-particle Hamiltonian for the collective motion

$$H=\frac{1}{N}(-i\partial_u - Na_0)^2 + N\sum_{\mu>0} v_{\mu N} e^{i\mu N u}(-1)^{\mu(N+1)} + \text{c.c.}$$

The relative ground state being the most symmetric, it follows from the periodicity and the antisymmetry (26) that the solutions to the Schrödinger equation must satisfy

$$\Psi\left(u+\frac{2\pi}{N}\right)=(-1)^{N-1}\Psi(u),$$

and that they are superpositions of functions of the type

$$\psi_k(u)=e^{iku}, \quad k=\begin{cases} \mu N & \text{if } N \text{ is odd} \\ \left(\mu+\frac{1}{2}\right)N & \text{if } N \text{ is even} \end{cases} \quad \mu\in\mathbb{Z}.$$

VII. CONCLUSIONS

We have investigated the electronic spectrum for a one-dimensional mesoscopic loop in a time-independent magnetic flux, admitting for an arbitrary number N of interacting electrons as well as for the presence of a one-particle potential.

Our approach for interacting electrons relies on the choice of an adequate basis of antisymmetric N-electron functions. Basis functions separable with respect to the collective and the relative motions are particularly convenient to treat the e-e interaction, since the latter depends only on the interelectronic distances. The best functions are the eigenfunctions of the Hamiltonian $H=H_0+H_{ee}$ for a zero one-particle potential, since they account already for the e-e interaction. For large e-e interaction parameters η^2, the interaction can be adequately treated in the harmonic approximation, where the relative motion of the electrons is described by $N-1$ harmonic oscillators. The excitation energies associated with the relative motion are proportional to η. The total-energy spectrum is obtained by summing the collective and the relative contributions. Following this approach, we have obtained a concise and transparent description of the ground state as well as of the first excited levels. The presented solutions become exact for strong e-e interaction.

Furthermore, we have investigated the interplay between the e-e interaction and the backscattering by a one-particle potential. The influence of both types of interaction on the persistent angular momentum (or persistent current), which is fully determined by the collective electronic motion in the ground state, has been discussed in detail. In agreement with Refs. 1,2, we find that the persistent angular momentum as well as the ground-state energy are both periodic in the magnetic flux with period $\Phi_0=h/e$. In absence of a one-particle potential term H_{eV}, the collective and relative motions are not coupled, and the persistent angular momentum remains equal to the free-electron value. The situation becomes different in presence of backscattering by a one-particle potential term H_{eV}, since the latter introduces a coupling between the relative and the collective electronic motions. The number of basis states needed to describe the N-electron states with lowest energies remains comfortably small for moderate one-particle potentials. We have shown that only the first Fourier components v_ν of H_{eV}, for example, $\nu=1,2,3$, and the Nth component v_N can be expected to lead to noteworthy coupling between the low-energy basis states. In agreement with the general findings of Ref. 20, we have further found that the e-e interaction tends to suppress the backscattering.[28] Our present analysis shows, however, that the suppression concerns only Fourier components with non-integer ν/N. Thus, in the limit $\eta^2\to\infty$, only the Fourier components $v_{\mu N}$, $\mu\in\mathbb{N}$, affect the collective motion and may reduce the persistent angular momentum with respect to the free-electron case. Considering the fact that the impurity potentials leading to backscattering have a limited range in the reciprocal space (or the ν space), we believe that this may explain that unexpected large persistent currents are found only for metallic loop structures, where N is large,[5,6] whereas the currents found in semiconductor ring systems appear to be of the expected order of magnitude.[7]

We have restricted our discussion to spinless electrons. The theoretical description can be extended to include spin wave functions. The energy spectra remain the same besides a shift in the magnetic flux by a multiple of Φ_0/N, depending on the symmetry of the spin function (see Ref. 29). Thus, admitting that the spin function changes to minimize the ground-state energy, we obtain oscillations of the ground-state energy and the persistent angular momentum with period Φ_0/N. This type of behavior is also found in descriptions based on the Hubbard model, see, e.g., Ref. 17.

In this work we have concentrated on the discussion of the ground-state properties, which are manifest in the persistent angular momenta. We did not fully exploit the achieved knowledge about the excited electronic states. In particular the low-energy excitations, which are well within the scope of the presented approach, are important for the understanding of the dynamical response properties of the considered ring system with respect to external time-dependent fields. The investigation of these features is presently underway.

ACKNOWLEDGMENT

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APPENDIX A: HARMONIC OSCILLATOR

The Hamiltonian for a particle in a one-dimensional parabolic potential is

$$H=-\frac{\hbar^2}{2m}\partial_x^2+\frac{m\omega^2}{2}x^2.$$

Its eigenvalues and eigenfunctions are

$$\mathcal{E}_n=\hbar\omega\left(n+\frac{1}{2}\right),\quad n\in\mathbb{N},$$

$$\varphi_n(x)=\frac{1}{\sqrt{x_0}\sqrt{2^n n!\sqrt{\pi}}}H_n(x/x_0)e^{-x^2/2x_0^2},\quad x_0=\sqrt{\frac{\hbar}{m\omega}},$$

where $H_n(z)$ is the nth Hermite polynomial. For $\hbar=2$ and $m=2$ we get the normalized Hamiltonian

$$H=-\partial_x^2+\omega^2x^2$$

with the eigenvalues and eigenfunctions

$$\mathcal{E}_n=2\omega\left(n+\frac{1}{2}\right),\quad n\in\mathbb{N},$$

$$\varphi_n(x)=\frac{\omega^{1/4}}{\sqrt{2^n n!\sqrt{\pi}}}H_n(x\sqrt{\omega})e^{-x^2\omega/2}. \tag{A1}$$

Accordingly, the Hamiltonian of the anisotropic harmonic oscillator in D dimensions is

$$H=-\Delta_D+\sum_{j=1}^{D}\omega_j^2q_j^2$$

with the eigenvalues and eigenfunctions

$$\mathcal{E}_{n_1,\ldots,n_D}=\sum_{j=1}^{D}\mathcal{E}_{n_j},$$

$$\mathcal{E}_{n_j}=2\omega_j\left(n_j+\frac{1}{2}\right)\quad n_j\in\mathbb{N},$$

$$\varphi_{n_1,\ldots,n_D}(\vec{q})=\prod_{j=1}^{D}\varphi_{n_j}(q_j),$$

$$\varphi_{n_j}(q_j)=\frac{\omega_j^{1/4}}{\sqrt{2^{n_j}n_j!\sqrt{\pi}}}H_{n_j}(q_j\sqrt{\omega})e^{-q_j^2\omega_j/2}.$$

For a particle in a two-dimensional isotropic parabolic potential $V(r)=\omega^2r^2$, the Hamiltonian of the harmonic oscillator expressed in polar coordinates reads

$$H=-\Delta+\omega^2r^2,\quad \Delta=\partial_r^2+\frac{1}{r}\partial_r+\frac{1}{r^2}\partial_\beta^2.$$

The eigenstates are obtained from

$$H\varphi(r,\beta)=\mathcal{E}\varphi(r,\beta)$$

with the boundary conditions

$$\varphi(r,\beta)=\varphi(r,\beta+2\pi),$$

$$\lim_{r\to\infty}\varphi(r,\beta)=0,$$

$$\lim_{r\to 0}\varphi(r,\beta)<\infty.$$

Separating the variables, we write

$$\varphi(r,\beta)=R(r)g(\beta),$$

where

$$g_l''(\beta)=-l^2g_l(\beta),\quad g_l(\beta)=\frac{1}{\sqrt{2\pi}}e^{il\beta},\ l\in\mathbb{Z},$$

and

$$-R''-\frac{1}{r}R'+\frac{l^2}{r^2}R+\omega^2r^2R=\mathcal{E}R,$$

with the boundary conditions $\lim_{r\to\infty}R(r)=0$ and $\lim_{r\to 0}R(r)<\infty$. Using the transformation $R(r)=r^{-1/2}f(r)$, we get finally the normalized solution[30]

$$\mathcal{E}_{ml}=2\omega(2m+|l|+1),\quad m\in\mathbb{N},\ l\in\mathbb{Z},$$

$$\varphi_{ml}(r,\beta)=R_{ml}(r)g_l(\beta), \tag{A2}$$

$$g_l(\beta)=\frac{1}{\sqrt{2\pi}}e^{il\beta},$$

$$R_{ml}(r)=\sqrt{2\omega}\left(\frac{m!}{(m+|l|)!}\right)^{1/2}(\sqrt{\omega}r)^{|l|}L_m^{(|l|)}(\omega r^2)e^{-\omega r^2/2},$$

where $L_m^{(\alpha)}(z)$ is the generalized Laguerre polynomial. We have

$$\int_{\mathbb{R}^2}|\varphi(x,y)|^2dx\,dy=\int_0^{2\pi}d\beta\int_0^{\infty}dr\,r|\varphi(r,\beta)|^2=1.$$

For a particle in a D-dimensional parabolic potential and even D, the potential may be described by a sum of two-dimensional isotropic parabolic potentials. Thus, the wave function for the harmonic oscillator can be written as a tensor product of solutions of type (A2). Accordingly, for odd dimensions *D*, the solution for the harmonic oscillator is given by a tensor product of $N-1$ solutions of type (A2) and one solution of type (A1).

APPENDIX B: ORTHOGONAL TRANSFORMATION IN REAL SPACE

The matrix P of the orthogonal transformation is given by

$$\begin{pmatrix} u \\ \vec{c} \end{pmatrix} = P\,\vec{\theta}, \quad P = \begin{pmatrix} 1/N & \cdots & 1/N & \cdots & 1/N \\ \vec{f}_1 & \cdots & \vec{f}_n & \cdots & \vec{f}_N \end{pmatrix}.$$

From the direct calculation $PP^t = D = \mathrm{diag}(1/N, 1, \dots, 1)$, one gets $D^{-1/2}PP^tD^{-1/2} = \mathbb{I}$, i.e., the matrix $U = D^{-1/2}P$ is unitary. Thus $UU^t = U^tU = P^tD^{-1}P = \mathbb{I}$. It follows

$$\vec{f}_n \cdot \vec{f}_{n'} + \frac{1}{N} = \delta_n^{n'},$$

$$\sum_{n=1}^{N} \vec{f}_n = \vec{0},$$

$$(\vec{f}_n - \vec{f}_{n'}) \cdot \vec{f}_{n''} = 0, \quad n \neq n'' \neq n',$$

$$(\vec{f}_n - \vec{f}_{n'}) \cdot \vec{f}_n = 1, \quad n \neq n',$$

$$\|(\vec{f}_n - \vec{f}_{n'})\|^2 = 2, \quad n \neq n'.$$

From the inverse relation

$$\vec{\theta} = P^{-1} \begin{pmatrix} u \\ \vec{c} \end{pmatrix},$$

it follows that each electron position can be written as

$$\theta_n = u + \vec{f}_n^{\,t} \vec{c}, \qquad n = 1, \dots, N.$$

For $n = 1, \dots, N$, the derivatives transform as

$$\partial_n = \partial_n u \, \partial_u + \sum_{j=1}^{N-1} \partial_n c_j \, \partial_{c_j} = \begin{pmatrix} \partial_n u \\ \partial_n \vec{c} \end{pmatrix}^t \begin{pmatrix} \partial_u \\ \partial_{c_1} \\ \vdots \\ \partial_{c_{N-1}} \end{pmatrix}$$

and formally as

$$\begin{pmatrix} \partial_1 \\ \vdots \\ \partial_N \end{pmatrix} = P^t \begin{pmatrix} \partial_u \\ \partial_{c_1} \\ \vdots \\ \partial_{c_{N-1}} \end{pmatrix}.$$

It follows

$$\sum_{n=1}^{N} \partial_n = \begin{pmatrix} 1 \\ \vdots \\ 1 \end{pmatrix}^t \begin{pmatrix} \partial_1 \\ \vdots \\ \partial_N \end{pmatrix} = \partial_u$$

and

$$\sum_{n=1}^{N} \partial_n^2 = \begin{pmatrix} \partial_1 \\ \vdots \\ \partial_N \end{pmatrix}^t \begin{pmatrix} \partial_1 \\ \vdots \\ \partial_N \end{pmatrix} = \frac{1}{N} \partial_u^2 + \Delta_{N-1},$$

$\Delta_{N-1} = \Sigma_{j=1}^{N-1} \partial_{c_j}^2$ being the Laplacian in $\mathbb{R}^{N-1}$.

APPENDIX C: HARMONIC APPROXIMATION

The *e*-*e* interaction potential is written as

$$H_{ee} = \eta^2 W,$$

with

$$W = \sum_{1 \leqslant n < n' \leqslant N} \frac{1}{\sin\left[\frac{1}{2}(\vec{f}_n^{\,t} - \vec{f}_{n'}^{\,t})(\vec{\Omega} + \vec{q})\right]}.$$

In second-order approximation we have

$$W \approx W_0 + W_1 + W_2.$$

The constant term is

$$W_0 = \sum_{1 \leqslant n < n' \leqslant N} \frac{1}{\sin a_{nn'}}.$$

The first-order term cancels, since

$$W_1 = -\frac{1}{2} \sum_{1 \leqslant n < n' \leqslant N} \frac{\cos a_{nn'}}{\sin^2 a_{nn'}} (\vec{f}_n^{\,t} - \vec{f}_{n'}^{\,t}) \vec{q}$$

$$= -\frac{1}{2} \sum_{\nu=1}^{N-1} \frac{\cos \frac{\nu\pi}{N}}{\sin^2 \frac{\nu\pi}{N}} \sum_{n=1}^{N-\nu} (\vec{f}_n^{\,t} - \vec{f}_{n+\nu}^{\,t}) \vec{q}$$

$$= -\frac{1}{4} \left(\sum_{\nu=1}^{N-1} \frac{\cos \frac{\nu\pi}{N}}{\sin^2 \frac{\nu\pi}{N}} \sum_{n=1}^{N-\nu} (\vec{f}_n^{\,t} - \vec{f}_{n+\nu}^{\,t}) - \sum_{\mu=1}^{N-1} \frac{\cos \frac{\mu\pi}{N}}{\sin^2 \frac{\mu\pi}{N}} \sum_{n=1}^{\mu} (\vec{f}_n^{\,t} - \vec{f}_{n+N-\mu}^{\,t}) \right) \vec{q}$$

$$= -\frac{1}{4} \sum_{\nu=1}^{N-1} \frac{\cos \frac{\nu\pi}{N}}{\sin^2 \frac{\nu\pi}{N}}$$

$$\times\left(\sum_{n=1}^{N-\nu}(\vec{f}_n^t-\vec{f}_{n+\nu}^t)-\sum_{n=1}^{\nu}(\vec{f}_n^t-\vec{f}_{n+N-\nu}^t)\right)\vec{q}=0.$$

The second-order term may be written as

$$W_2=\vec{q}^{\,t}M\vec{q},$$

with the symmetric bilinear form in $\mathbb{R}^{N-1}$

$$M=\sum_{1\leqslant n<n'\leqslant N}\frac{1+\cos^2 a_{nn'}}{8\sin^3 a_{nn'}}(\vec{f}_n-\vec{f}_{n'})(\vec{f}_n^t-\vec{f}_{n'}^t).$$

The matrix elements of M are

$$M_{ij}=\sum_{1\leqslant n<n'\leqslant N}\frac{1+\cos^2 a_{nn'}}{8\sin^3 a_{nn'}}(\vec{f}_n-\vec{f}_{n'})_i(\vec{f}_n-\vec{f}_{n'})_j\,.$$

For $j=1,\dots,N-1$ one has

$$(\vec{f}_n-\vec{f}_{n'})_j=\frac{\sqrt{2}}{\sqrt{N}}\left[\cos\left(jn\beta_0+\frac{\pi}{4}\right)-\cos\left(jn'\beta_0+\frac{\pi}{4}\right)\right]$$

$$=2\frac{\sqrt{2}}{\sqrt{N}}\sin\frac{\nu j\beta_0}{2}\cos\frac{\mu j\beta_0}{2},$$

with $\nu=n'-n$, and $\mu=n'+n$ having same parity. The double sum transforms as

$$\sum_{1\leqslant n<n'\leqslant N}\cdots=\frac{1}{2}\sum_{\nu=1}^{N-1}\sum_{\mu=1}^{2N}{}^{(\nu)}\cdots,$$

where $\Sigma^{(\nu)}$ extends over μ values having the same parity as ν. Moreover, the identity

$$\sum_{\mu=1}^{2N}{}'\cos\frac{\mu i\beta_0}{2}\cos\frac{\mu j\beta_0}{2}=\frac{N}{2}\delta_{ij}\,,$$

the sum Σ' extending over either odd or even values, leads finally to the diagonal form

$$M_{ij}=\omega_j^2\delta_{ij}\,,$$

with

$$\omega_j^2=\sum_{\nu=1}^{N-1}\frac{1+\cos^2\dfrac{\nu\pi}{N}}{4\sin^3\dfrac{\nu\pi}{N}}\sin^2\frac{j\nu\pi}{N},\quad j=1,\dots,N-1.$$

The smallest frequencies are given by

$$\omega_{N-1}^2=\omega_1^2=\frac{1}{2}\left(\sum_{\nu=1}^{N-1}\frac{1}{\sin\dfrac{\nu\pi}{N}}-\frac{1}{2}\cot\frac{\pi}{2N}\right).$$

For large (but, because of the divergence of $1/\sin x$ at $x=0$ and $x=\pi$, not too large) N, the sum may be approximated by an integral,

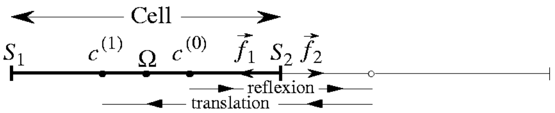

FIG. 12. $N=2$. Cell and symmetries in $\mathbb{R}$.

$$\omega_1^2\approx\frac{1}{2}\left(\frac{N}{\pi}\int_{\pi/2N}^{\pi-(\pi/2N)}\frac{dx}{\sin x}-\frac{1}{2}\cot\frac{\pi}{2N}\right)$$

$$\approx\frac{N}{\pi}\ln\frac{4N}{\pi\sqrt{\exp(1)}}.$$

APPENDIX D: EXAMPLES

(1) N=2. The collective and relative positions are

$$u=\frac{1}{2}(\theta_1+\theta_2),\quad c=\theta_1 f_1+\theta_2 f_2,$$

with

$$f_1=-\frac{1}{\sqrt{2}},\quad f_2=\frac{1}{\sqrt{2}}.$$

The particular cell $C\subset\mathbb{R}$ (Fig. 12) has the edges and the center

$$S_1=-\sqrt{2}\pi,\quad S_2=0,\quad \Omega=-\frac{\pi}{\sqrt{2}}.$$

With the shift of the origin to the center Ω, the symmetry of the wave function (26) becomes

$$\Psi(u',q')=-\Psi(u,q),$$

where

$$u'=u+\pi,\quad q'=-q.$$

For $H_{eV}=0$, the wave function is separable and the condition (30) gives

$$e^{ik\pi}\varphi(q')=-\varphi(q).$$

The energies of the stationary states are

$$E=\frac{1}{2}(k-2a_0)^2+\mathcal{E}_n\,,\ \ k\in\mathbb{Z}.$$

For the discussed cases of the e-e interaction, the energies $\mathcal{E}_n$ of the relative motion can be given explicitly (see also Fig. 2).

No interaction $\eta^2=0$:

$$\mathcal{E}_n=\frac{n^2}{2},\ \ n\geqslant 1,\ \ n\ \text{ same parity as }\ k.$$

Harmonic approximation $\eta^2\gg 1$: $\omega_1^2=\omega^2=\frac{1}{4}$,

$$\mathcal{E}_n=2\eta n\omega=n\eta,\ \ n\geqslant 0,\ \ n\ \text{ opposite parity as }\ k.$$

(2) N=3. The collective and relative positions are

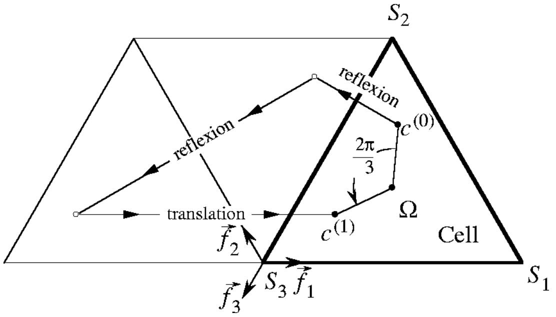

FIG. 13. $N=3$. Cell and symmetries in $\mathbb{R}^2$.

$$u=\frac{1}{3}(\theta_1+\theta_2+\theta_3),\quad \vec{c}=\theta_1\vec{f}_1+\theta_2\vec{f}_2+\theta_3\vec{f}_3$$

with

$$\vec{f}_1=\frac{1}{2\sqrt{3}}\begin{pmatrix}-1-\sqrt{3}\\-1+\sqrt{3}\end{pmatrix},\quad \vec{f}_2=\frac{1}{2\sqrt{3}}\begin{pmatrix}-1+\sqrt{3}\\-1-\sqrt{3}\end{pmatrix},$$

$$\vec{f}_3=\frac{1}{\sqrt{3}}\begin{pmatrix}1\\1\end{pmatrix}.$$

The particular cell $C\subset\mathbb{R}^2$ (Fig. 13) has the edges

$$\vec{S}_1=\frac{\pi}{\sqrt{3}}\begin{pmatrix}-1-\sqrt{3}\\-1+\sqrt{3}\end{pmatrix},\ \vec{S}_2=\frac{\pi}{\sqrt{3}}\begin{pmatrix}-2\\-2\end{pmatrix},\ \vec{S}_3=\vec{0},$$

and the center

$$\vec{\Omega}=\frac{\pi}{3\sqrt{3}}\begin{pmatrix}-3-\sqrt{3}\\-3+\sqrt{3}\end{pmatrix}.$$

With the shift of the origin to the center $\vec{\Omega}$, the symmetry of the wave function (26) becomes

$$\Psi(u',\vec{q}\,')=\Psi(u,\vec{q}),$$

with

$$u'=u+\frac{2\pi}{3},\quad \begin{pmatrix}q_1'\\q_2'\end{pmatrix}=R\left(\frac{2\pi}{3}\right)\begin{pmatrix}q_1\\q_2\end{pmatrix},$$

where the matrix $R(\beta)$ defines a rotation of angle β. For $H_{eV}=0$, the wave function is separable and the condition (30) gives

$$e^{ik(2\pi/3)}\varphi(\vec{q}\,')=\varphi(\vec{q}).$$

The energy of the stationary state is

$$E=\frac{1}{2}(k-2a_0)^2+\mathcal{E}_{n_1,n_2}.$$

For the discussed cases of the *e*-*e* interaction we obtain the following energy values.

No interaction $\eta^2=0$:

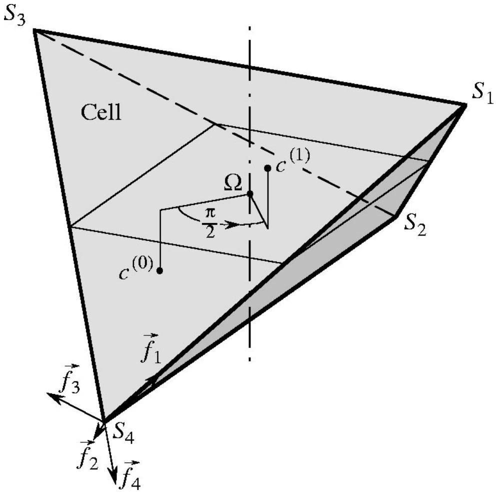

FIG. 14. $N=4$. Cell and symmetries in $\mathbb{R}^3$.

$$\mathcal{E}_{n_1,n_2}=\frac{2}{3}(n_1^2+n_1n_2+n_2^2),\ \ n_1,n_2\geqslant 1,$$

$$k=3\mu+2n_2+n_1.$$

This is the spectrum of the vibrating membrane on an equilateral triangle.

Harmonic approximation $\eta^2\gg 1$: $\omega_1^2=\omega_2^2=\omega^2=\frac{5}{4\sqrt{3}}$,

$$\mathcal{E}_{n_1,n_2}=2\eta\omega(n_1+n_2),\ \ n_1,n_2\geqslant 0,$$

$$k=3\mu-n_1-2n_2.$$

(3) N=4. The collective and relative positions are

$$u=\frac{1}{4}(\theta_1+\theta_2+\theta_3+\theta_4),\ \ \vec{c}=\theta_1\vec{f}_1+\theta_2\vec{f}_2+\theta_3\vec{f}_3+\theta_4\vec{f}_4$$

with

$$\vec{f}_1=\frac{1}{2}\begin{pmatrix}-1\\-1\\1\end{pmatrix},\ \vec{f}_2=\frac{1}{2}\begin{pmatrix}-1\\1\\-1\end{pmatrix},$$

$$\vec{f}_3=\frac{1}{2}\begin{pmatrix}1\\-1\\-1\end{pmatrix},\ \vec{f}_4=\frac{1}{2}\begin{pmatrix}1\\1\\1\end{pmatrix}.$$

The particular cell $C\subset\mathbb{R}^3$ (Fig. 14) has the edges

$$\vec{S}_1=\pi\begin{pmatrix}-1\\-1\\1\end{pmatrix},\ \vec{S}_2=\pi\begin{pmatrix}-2\\0\\0\end{pmatrix},$$

$$\vec{S}_3=\pi\begin{pmatrix}-1\\-1\\-1\end{pmatrix},\ \vec{S}_4=\vec{0},$$

TABLE II. Values for $A_{ml}^{m'l'}(z)$.

$A_{ml}^{m'l'}(z)$	(0,0)	$(0,-1)$	(0,1)	$(0,-2)$	(1,0)	(0,2)
(0,0)	1	z	$-z$	$\frac{z^2}{\sqrt{2}}$	z^2	$\frac{z^2}{\sqrt{2}}$
$(0,-1)$	$-z$	$1-z^2$	z^2	$-\frac{z(-2+z^2)}{\sqrt{2}}$	$z(1-z^2)$	$-\frac{z^3}{\sqrt{2}}$
(0,1)	z	z^2	$1-z^2$	$\frac{z^3}{\sqrt{2}}$	$-z(1-z^2)$	$\frac{z(-2+z^2)}{\sqrt{2}}$
$(0,-2)$	$\frac{z^2}{\sqrt{2}}$	$\frac{z(-2+z^2)}{\sqrt{2}}$	$-\frac{z^3}{\sqrt{2}}$	$\frac{2-4z^2+z^4}{2}$	$\frac{z^2(-2+z^2)}{\sqrt{2}}$	$\frac{z^4}{2}$
(1,0)	z^2	$-z(1-z^2)$	$z(1-z^2)$	$\frac{z^2(-2+z^2)}{\sqrt{2}}$	$(1-z^2)^2$	$\frac{z^2(-2+z^2)}{\sqrt{2}}$
(0,2)	$\frac{z^2}{\sqrt{2}}$	$\frac{z^3}{\sqrt{2}}$	$-\frac{z(-2+z^2)}{\sqrt{2}}$	$\frac{z^4}{2}$	$\frac{z^2(-2+z^2)}{\sqrt{2}}$	$\frac{2-4z^2+z^4}{2}$

and the center

$$\vec{\Omega}=\frac{\pi}{2}\begin{pmatrix}-2\\-1\\0\end{pmatrix}.$$

With the shift of the origin to the center $\vec{\Omega}$, the symmetry of the wave function (26) becomes

$$\Psi(u',\vec{q}\,')=-\Psi(u,\vec{q}),$$

where

$$u'=u+\frac{\pi}{2},\quad \begin{pmatrix}q_1'\\q_3'\end{pmatrix}=R\left(\frac{\pi}{2}\right)\begin{pmatrix}q_1\\q_3\end{pmatrix},\quad q_2'=-q_2.$$

For $H_{eV}=0$, the wave function is separable and the condition (30) gives

$$e^{ik(\pi/2)}\varphi(\vec{q}\,')=-\varphi(\vec{q}).$$

The energy of the stationary state is

$$E=\frac{1}{2}(k-2a_0)^2+\mathcal{E}_{n_1,n_2,n_3}.$$

For the discussed cases of the e-e interaction we obtain the following energy values.

No interaction $\eta^2=0$:

$$\mathcal{E}_{n_1,n_2,n_3}=\frac{1}{4}[n_1^2+n_2^2+n_3^2+(n_1+n_2)^2+(n_2+n_3)^2+(n_1+n_2+n_3)^2],$$

$$k=4\mu+3n_3+2n_2+n_1,$$

with $n_1,n_2,n_3\geqslant 1$.

Harmonic approximation $\eta^2\gg 1$: $\omega_1^2=\omega_3^2=\frac{3\sqrt{2}+1}{4}$, $\omega_2^2=\frac{3\sqrt{2}}{2}$,

$$\mathcal{E}_{n_1,n_2,n_3}=2\eta(\omega_1 n_1+\omega_2 n_2+\omega_3 n_3),$$

$$k=4\left(\mu+\frac{1}{2}\right)-n_1-2n_2-3n_3,$$

with $n_1,n_2,n_3\geqslant 0$.

APPENDIX E: MATRIX ELEMENTS FOR THE *N*-ELECTRON CASE

We have to determine the matrix elements

$$\langle\varrho|I_\nu|\varrho'\rangle=\sum_{n=1}^{N}\exp\left(i\nu\frac{\pi}{N}(N+1-2n)\right)\times\prod_{j=1}^{(N-1)/2}\langle ml|\exp\left(i\nu\frac{\sqrt{2}}{\sqrt{N}}r\sin(\beta+\alpha_n)\right)|m'l'\rangle_j,$$

with $\alpha_n=\pi/4-nj\beta_0$ for all j. The transformations $\phi=\beta+\alpha_n$ and $x=\sqrt{\eta\omega}r$ yield

$$\langle ml|\exp\left(i\nu\frac{\sqrt{2}}{\sqrt{N}}r\sin(\beta+\alpha_n)\right)|m'l'\rangle=\frac{1}{2\pi}\int_0^{2\pi}d\beta\int_0^{\infty}dr\,rR_{ml}(r)R_{m'l'}(r)e^{i(l-l')\beta}\times\exp\left(i\nu\frac{\sqrt{2}}{\sqrt{N}}r\sin(\beta+\alpha_n)\right)=e^{i(l-l')\alpha_n}e^{-z_\nu^2}A_{ml}^{m'l'}(z_\nu),$$

TABLE III. Fourier component of H_{eV} coupling the states $|\varrho\rangle$.

ν	$\|0\rangle$	$\|1^{+1}\rangle$	$\|1^{-1}\rangle$	$\|1^{+2}\rangle$	$\|1^{-2}\rangle$	$\|2^{+1}\rangle$	$\|2^{0}\rangle$	$\|2^{-1}\rangle$
$\langle 0\|$	$\pm N$	1	-1	2	-2	2	$\pm N$	-2
$\langle 1^{+1}\|$	-1	$\pm N$	-2	1	-3	1	-1	-3
$\langle 1^{-1}\|$	1	2	$\pm N$	3	-1	3	1	-1
$\langle 1^{+2}\|$	-2	-1	-3	$\pm N$	-4	$\pm N$	-2	-4
$\langle 1^{-2}\|$	2	3	1	4	$\pm N$	4	2	$\pm N$
$\langle 2^{+1}\|$	-2	-1	-3	$\pm N$	-4	$\pm N$	-2	-4
$\langle 2^{0}\|$	$\pm N$	1	-1	2	-2	2	$\pm N$	-2
$\langle 2^{-1}\|$	2	3	1	4	$\pm N$	4	2	$\pm N$

where $z_\nu = z_{\nu j} = \nu/\sqrt{2N\eta\omega_j}$ and

$$e^{-z^2}A_{ml}^{m'l'}(z) = \left(\frac{m!\,m'!}{(m+|l|)!\,(m'+|l'|)!}\right)^{1/2} \cdot \int_0^\infty dx\, 2x^{|l|+|l'|+1} J_{l-l'}(2zx) L_m^{(|l|)}(x^2) L_{m'}^{(|l'|)}(x^2) e^{-x^2}.$$

The values for $A_{m\ell}^{m'\ell'}(z)$ are given in Table II. Including the index j, we get

$$\langle\varrho|I_\nu|\varrho'\rangle = \sum_{n=1}^{N} \exp\left(i\nu\frac{\pi}{N}(N+1-2n)\right) \times \prod_{j=1}^{(N-1)/2} e^{i[(l_j-l_j')\alpha_{nj}e_{vj}^{-z^2}]}A_{m_jl_j}^{m_j'l_j'}(z_{\nu j})$$

$$= e^{i\nu[(N+1)\pi/N]}J_\nu \times \sum_{n=1}^{N} \exp\left\{-i\left[\nu + \sum_{j'} (l_{j'}-l_{j'}')j'\right]n\beta_0\right\} \times \prod_{j=1}^{(N-1)/2} e^{i(l_j-l_j')(\pi/4)}A_{m_jl_j}^{m_j'l_j'}(z_{\nu j})$$

where

$$J_\nu = \prod_{j=1}^{(N-1)/2} e^{-z_{\nu j}^2} = \exp\left(-\frac{\nu^2}{2N\eta}\sum_{j=1}^{(N-1)/2}\frac{1}{\omega_j}\right).$$

Evaluating the sum over n, which determines the coupling due to the Fourier component v_ν, we get finally

$$\langle\varrho|I_\nu|\varrho'\rangle = \begin{cases} Ne^{i\nu[(N+1)\pi/N]}J_\nu \displaystyle\prod_{j=1}^{(N-1)/2} e^{i(l_j-l_j')(\pi/4)}A_{m_jl_j}^{m_j'l_j'}(z_{\nu j}) \\ \quad \text{if } \nu + \displaystyle\sum_{j'=1}^{(N-1)/2}(l_{j'}-l_{j'}')j' = \mu N, \\ 0 \quad \text{otherwise.} \end{cases}$$

The Fourier components v_ν leading to coupling between states $|\varrho\rangle$ are resumed in Table III.

As already pointed out before, each relative excitation $\mathcal{E}_\varrho$ corresponds to a set of parabolic energy bands in a_0 with minima at energy $\mathcal{E}_\varrho$. Figure 15 shows the lowest excitation energies $\mathcal{E}_\varrho$ of the relative motion as a function of the number of electrons N.

For $N \geqslant 11$, the four lowest excitations are

$$\mathcal{E}_0 = 0 < \mathcal{E}_1^{(1)} = 2\eta\omega_1 < \mathcal{E}_1^{(2)} = 2\eta\omega_2 < \mathcal{E}_2^{(1)} = 4\eta\omega_1,$$

where the superscript (j) denotes the oscillator, and the subscript n its excitation level. Indeed, for large N one has

$$0 < 4\omega_1^2 - \omega_2^2 = \eta^2 \frac{3\cos\dfrac{3\pi}{2N} + 5\cos\dfrac{\pi}{2N}}{2\sin\dfrac{3\pi}{2N}} \approx \eta^2\frac{8N}{3\pi}.$$

Moreover, we have obviously $\mathcal{E}_2^{(1)} < \mathcal{E}_1^{(1)} + \mathcal{E}_1^{(2)}$ and also $\mathcal{E}_2^{(1)} < \mathcal{E}_1^{(3)} = 2\eta\omega_3$, since

$$0 < \omega_3^2 - 4\omega_1^2 \approx \eta^2\frac{N}{\pi}\left(5\ln\frac{4N}{\pi\sqrt{\exp(1)}} - \frac{122}{15}\right).$$

The distance $\mathcal{E}_1^{(3)} - \mathcal{E}_2^{(1)}$ increases faster with N than $\mathcal{E}_2^{(1)} - \mathcal{E}_1^{(2)}$. A good choice is thus to consider only the relative ground state $\mathcal{E}_0$ and the three first relative excitations $\mathcal{E}_1^{(1)}$, $\mathcal{E}_1^{(2)}$, and $\mathcal{E}_2^{(1)}$ in the numerical calculations.

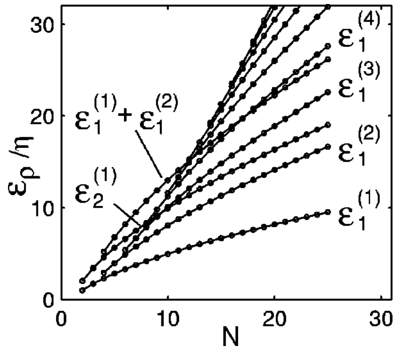

FIG. 15. Excitation energies $\mathcal{E}_\varrho$ associated with the relative motion as a function of the number of electrons N: single-mode excitation energies $\mathcal{E}_1^{(j)}$ of the oscillator modes j, and lowest double-excitation energies $\mathcal{E}_2^{(1)}$ and $\mathcal{E}_1^{(1)} + \mathcal{E}_1^{(2)}$. The lines are drawn as guides to the eye.

The nonzero matrix elements $\langle \varrho | I_\nu | \varrho' \rangle$ for $\nu = \pm N$ and $\nu = \pm 1$ are given below:

$$\langle 0 | I_{\pm N} | 0 \rangle = N J_N ,$$

$$\langle 1^{+1} | I_{\pm N} | 1^{+1} \rangle = N J_N A^{0,1}_{0,1}(z_{N1}) = N J_N (1 - z_{N1}^2),$$

$$\langle 1^{-1} | I_{\pm N} | 1^{-1} \rangle = N J_N A^{0,-1}_{0,-1}(z_{N1}) = N J_N (1 - z_{N1}^2),$$

$$\langle 1^{+2} | I_{\pm N} | 1^{+2} \rangle = N J_N A^{0,1}_{0,1}(z_{N2}) = N J_N (1 - z_{N2}^2),$$

$$\langle 1^{-2} | I_{\pm N} | 1^{-2} \rangle = N J_N A^{0,-1}_{0,-1}(z_{N2}) = N J_N (1 - z_{N2}^2),$$

$$\langle 2^{+1} | I_{\pm N} | 2^{+1} \rangle = N J_N A^{0,2}_{0,2}(z_{N1}) = N J_N \frac{1}{2}(2 - 4 z_{N1}^2 + z_{N1}^4),$$

$$\langle 2^{0} | I_{\pm N} | 2^{0} \rangle = N J_N A^{1,0}_{1,0}(z_{N1}) = N J_N (1 - z_{N1}^2)^2,$$

$$\langle 2^{-1} | I_{\pm N} | 2^{-1} \rangle = N J_N A^{0,-2}_{0,-2}(z_{N1}) = N J_N \frac{1}{2}(2 - 4 z_{N1}^2 + z_{N1}^4),$$

$$\langle 0 | I_{\pm N} | 2^{0} \rangle = N J_N A^{1,0}_{0,0}(z_{N1}) = N J_N z_{N1}^2 ,$$

$$\langle 2^{0} | I_{\pm N} | 0 \rangle = N J_N A^{0,0}_{1,0}(z_{N1}) = N J_N z_{N1}^2 ,$$

$$\langle 1^{+2} | I_{\pm N} | 2^{+1} \rangle = N J_N e^{-i(\pi/4)} A^{0,2}_{0,0}(\pm z_{N1}) A^{0,0}_{0,1}(\pm z_{N2})$$

$$= \pm e^{-i(\pi/4)} N J_N \frac{1}{\sqrt{2}} z_{N1}^2 z_{N2} ,$$

$$\langle 2^{+1} | I_{\pm N} | 1^{+2} \rangle = N J_N e^{i(\pi/4)} A^{0,0}_{0,2}(\pm z_{N1}) A^{0,1}_{0,0}(\pm z_{N2})$$

$$= \mp e^{i(\pi/4)} N J_N \frac{1}{\sqrt{2}} z_{N1}^2 z_{N2} ,$$

$$\langle 1^{-2} | I_{\pm N} | 2^{-1} \rangle = N J_N e^{i(\pi/4)} A^{0,-2}_{0,0}(\pm z_{N1}) A^{0,0}_{0,-1}(\pm z_{N2})$$

$$= \mp e^{i(\pi/4)} N J_N \frac{1}{\sqrt{2}} z_{N1}^2 z_{N2} ,$$

$$\langle 2^{-1} | I_{\pm N} | 1^{-2} \rangle = N J_N e^{-i(\pi/4)} A^{0,0}_{0,-2}(\pm z_{N1}) A^{0,-1}_{0,0}(\pm z_{N2})$$

$$= \pm e^{-i(\pi/4)} N J_N \frac{1}{\sqrt{2}} z_{N1}^2 z_{N2} ,$$

$$\langle 0 | I_1 | 1^{+1} \rangle = \overline{\langle 1^{+1} | I_{-1} | 0 \rangle} = e^{i(\pi/N - \pi/4)} N J_1 z_{11} ,$$

$$\langle 1^{-1} | I_1 | 0 \rangle = \overline{\langle 0 | I_{-1} | 1^{-1} \rangle} = e^{i(\pi/N - \pi/4)} N J_1 z_{11} ,$$

$$\langle 1^{+1} | I_1 | 1^{+2} \rangle = \overline{\langle 1^{+2} | I_{-1} | 1^{+1} \rangle} = e^{i(\pi/N)} N J_1 z_{11} z_{12} ,$$

$$\langle 1^{+1} | I_1 | 2^{+1} \rangle = \overline{\langle 2^{+1} | I_{-1} | 1^{+1} \rangle}$$

$$= - e^{i(\pi/N - \pi/4)} N J_1 \frac{1}{\sqrt{2}} z_{11}(-2 + z_{11}^2),$$

$$\langle 2^{0} | I_1 | 1^{+1} \rangle = \overline{\langle 1^{+1} | I_{-1} | 2^{0} \rangle} = - e^{i(\pi/N - \pi/4)} N J_1 z_{11}(1 - z_{11}^2),$$

$$\langle 1^{-2} | I_1 | 1^{-1} \rangle = \overline{\langle 1^{-1} | I_{-1} | 1^{-2} \rangle} = e^{i\pi/N} N J_1 z_{11} z_{12} ,$$

$$\langle 1^{-1} | I_1 | 2^{0} \rangle = \overline{\langle 2^{0} | I_{-1} | 1^{-1} \rangle} = - e^{i(\pi/N - \pi/4)} N J_1 z_{11}(1 - z_{11}^2),$$

$$\langle 2^{-1} | I_1 | 1^{-1} \rangle = \overline{\langle 1^{-1} | I_{-1} | 2^{-1} \rangle}$$

$$= - e^{i(\pi/N - \pi/4)} N J_1 \frac{1}{\sqrt{2}} z_{11}(-2 + z_{11}^2).$$

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[28] The systematic decrease of the persistent current in the large-interaction limit found by Ref. 16 results from the fact that the band width of one-electron spectrum is assumed to be *finite* in the Hubbard model employed there. In this case, the one-electron Hamiltonian becomes negligible in the large-interaction limit, so that the system becomes a Mott insulator and the current is suppressed. This is in contrast with our presently used continuous real-space representation, which allows for arbitrary large one-electron energies.

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