One-particle Green’s function of interacting two electrons using analytic solutions for a three-body problem: comparison with exact Kohn–Sham system

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Received 15 August 2018, revised 12 September 2018
Accepted for publication 19 September 2018
Published 5 October 2018

Abstract

For a three-electron system with finite-strength interactions confined to a one-dimensional harmonic trap, we solve the Schrödinger equation analytically to obtain the exact solutions, from which we construct explicitly the simultaneous eigenstates of the energy and total spin for the first time. The solutions for the three-electron system allow us to derive analytic expressions for the exact one-particle Green’s function (GF) for the corresponding two-electron system. We calculate the GF in frequency domain to examine systematically its behavior depending on the electronic interactions. We also compare the pole structure of non-interacting GF using the exact Kohn–Sham (KS) potential with that of the exact GF to find that the discrepancy of the energy gap between the KS system and the original system is larger for a stronger interaction. We perform numerical examination on the behavior of GFs in real space to demonstrate that the exact and KS GFs can have shapes quite different from each other. Our simple model will help to understand generic characteristics of interacting GFs.

Keywords: Green’s functions, exactly solvable model, electronic correlation

(Some figures may appear in colour only in the online journal)
interacting system even if we knew the exact exchange correlation functional, it is useful to have a simple many-electron model which enables one to calculate the exact GF and compare it with the one constructed via the DFT calculation.

Photoelectron spectroscopy has become an active research field today. Measurements of photoelectron spectra performed in various ways such as angle-resolved photoemission spectroscopy (ARPES) for clarifying the properties of materials. The measured spectra are often explained under a certain assumption via the one-particle GF of a many-electron system [11–13]. The clear understanding of the characteristics of GFs is thus important not only for theoretical studies, but also for practical studies in material science. The calculation of GFs in the context of explicitly correlated electronic-structure calculations for realistic systems has been drawing attention recently [14–16].

Given the progresses on the theoretical and experimental studies outlined above, one notices that it is worth finding a new exactly solvable many-electron model in real space and proposing a minimal model for an exact interacting one-particle GF. In the present study, we obtain the exact solutions of the Schrödinger equation for a three-electron system with finite-strength interactions confined to a one-dimensional trap, from which we construct explicitly the simultaneous eigenstates of the energy and total spin for the first time, to our best knowledge. In addition, we provide the exact one-particle GF of the corresponding two-electron system and compare it with that in the KS system. Analytic solutions for an arbitrary number of confined spin-1/2 fermions with delta-type interactions in the strong-interaction limit have been obtained by employing a group-theoretic approach. [17] Numerical solutions for such fermions with particle numbers more than two have also been reported for finite-strength interactions [18]. There exist various theoretical studies on confined interacting particles in the context of one-dimensional Fermi gases [5].

This paper is organized as follows. In section 2, we provide the analytic solutions of the Schrödinger equation for the interacting three-electron system, from which we construct the eigenstates of the energy and total spin. In section 3, we derive the exact expressions for the one-particle GF of the two-electron system and perform numerical calculations to examine the behavior of the GFs. In section 4, the conclusions are provided.

### 2. Exact solutions of Schrödinger equations

#### 2.1. One-electron system

The Hamiltonian for an electron confined to a one-dimensional harmonic trap \( V_0(x) = m_e \omega_0^2 x^2 / 2 \) with its strength \( \omega_0 \) is \( H^{HO}(x; m_e, \omega_0) = -1 / (2m_e) \partial^2 / \partial x^2 + V_0(x) \). \( m_e \) is the electron mass. The orthonormalized eigenfunction is given by \( \psi_n(x) = \psi_n^{HO}(x; \ell / \omega_0) \equiv 1 / (\sqrt{2 \pi} \sqrt{m_e}) \exp(-\pi^2 / 4) H_n(x / \sqrt{2}) \), where \( \ell \equiv 1 / \sqrt{2m_e \omega_0} \) is the typical length scale and \( T_1 \equiv x / \ell \) is the dimensionless coordinate. \( H_n(x) \) is the Hermite polynomial. The energy eigenvalue for the quantum number \( n \) is \( E_n^{(1)} = \omega_0(n + 1 / 2) \), as found in textbooks of quantum mechanics. The corresponding wave function (WF) for an electron is given by \( \Psi_n^{(1)}(x_1, x_2) = \psi_n^{HO}(x_1 / \ell; \ell) \chi^{S=1/2,S} \), \( \chi^{S=1/2,S} \) is the spin WF with \( \chi^{S=1/2,1/2} = \beta(1) \).

#### 2.2. Two-electron system

The Hamiltonian for the confined interacting two electrons considered in the present work is

\[
H^{(2)} = H^{HO}(x_1; m_e, \omega_0) + H^{HO}(x_2; m_e, \omega_0) + v(x_1 - x_2),
\]

where

\[
v(x) = -\frac{m_e \omega_0^2 \Lambda}{2} x^2
\]

is the repulsive interaction between the electrons. The dimensionless parameter \( 0 \leq \Lambda \leq 1 / 3 \) measures the strength of interaction. This model has been studied intensively [19–22]. The variable transformation for the center-of-mass coordinate \( x_+ \equiv (x_1 + x_2) / 2 \) and the scaled relative coordinate \( x_- \equiv (x_1 - x_2) / \sqrt{2} \) decouples the interacting Hamiltonian into two Hamiltonians for independent harmonic oscillators as

\[
H^{(2)} = H^{HO}(x_+; M_2, \omega_0) + H^{HO}(x_-; m_e, \omega_0),
\]

where \( M_2 \equiv 2m_e \) and \( \omega_0 \equiv \sqrt{1 - 2 \Lambda \omega_0^2} \equiv \lambda \omega_0 \). The solution for the center-of-mass motion is \( \psi_{\Lambda n_\Lambda}(x_+) = \psi_{n_\Lambda}^{HO}(\sqrt{\Lambda} x_+ / \ell; \ell / \sqrt{2}) \) and that for the relative motion is \( \psi_{n_\Lambda}(x_-) = \psi_{n_\Lambda}^{HO}(\sqrt{\Lambda} x_- / \ell; \ell / \sqrt{2}) \). With the quantum numbers \( n_\Lambda \) and \( n_\Lambda \), the energy eigenvalue for the whole system is given simply by the sum of two energy eigenvalues for the two oscillators:

\[
E^{(2)}_{n_\Lambda n_\Lambda} = \omega_0 \left( n_\Lambda + \frac{1}{2} \right) + \lambda \omega_0 \left( n_\Lambda + \frac{1}{2} \right),
\]

whose corresponding normalized spatial WF is

\[
\Psi_{n_\Lambda n_\Lambda}(x_1, x_2) = 2^{1/4} \psi_{n_\Lambda}(x_+) \psi_{n_\Lambda}(x_-).
\]

The Fermi statistics forces the two-electron WFs for the energy eigenstates to be in the following two forms:

\[
\Psi_{n_\Lambda n_\Lambda}^{S=0}(x_1, x_2) = \Psi_{n_\Lambda n_\Lambda}(x_1, x_2) \chi_{0,0}^{S=0}(s_1, s_2)
\]

with an even \( n_\Lambda \) for a spin-singlet state and

\[
\Psi_{n_\Lambda n_\Lambda}^{S=1}(x_1, x_2) = \Psi_{n_\Lambda n_\Lambda}(x_1, x_2) \chi_{1,S}^{S=1}(s_1, s_2)
\]

with an odd \( n_\Lambda \) for spin-triplet states. \( \chi_{1,S}^{S=1}(s_1, s_2) \) is the spin WF for two electrons having the total spin \( S \) and its z component \( S_z \). The ground state is non-degenerate and its WF is given by

\[
\Psi_{g_s}^{(2)}(x_1, x_2, s_1, s_2) = \Psi_{S=0;S=0}^{S=0}(x_1, x_2, s_1, s_2)
\]

with the energy eigenvalue \( E_{g_s}^{(2)} = E_{g0}^{(2)} \).

#### 2.3. Three-electron system

#### 2.3.1. Variable transformations

Calogero [23] provided the exact analytic solutions for an interacting spinless three-particle system confined to a one-dimensional trap. In
the present study, we adopt his approach to obtain the solutions for a three-electron system necessary for deriving the expressions for the GF of the two-electron system.

The Hamiltonian for the interacting three-electron system we have to consider is

\[
H^{(3)} = H^{\text{HO}}(x_1; m_e, \omega_0) + H^{\text{HO}}(x_2; m_e, \omega_0) + \psi(x_1 - x_2) + \psi(x_2 - x_3) + \psi(x_3 - x_1). \tag{8}
\]

The energy eigenstates of this system are necessary for the calculation of GF for the two-electron system described above. The interactions considered by Calogero \[23\] was inverse-quadratic interactions in addition to those present in equation (8).

It is appropriate to perform the two successive variable transformations. The first one is \((x_1, x_2, x_3) \rightarrow (X, x, y)\):

\[
X \equiv \frac{1}{3} (x_1 + x_2 + x_3) \tag{9}
\]

\[
x \equiv \frac{1}{\sqrt{2}} (x_1 - x_2) \tag{10}
\]

\[
y \equiv \frac{1}{\sqrt{6}} (x_1 + x_2 - 2x_3), \tag{11}
\]

which are called the Jacobi coordinates. The second one is \((X, x, y) \rightarrow (X, r, \phi)\):

\[
r \equiv \sqrt{X^2 + y^2}, \tag{12}
\]

\[
\phi \equiv \begin{cases} \arctan \frac{y}{x} & (x \geq 0) \\ \arctan \frac{y}{x} + \pi & (x < 0) \end{cases}, \tag{13}
\]

where we define the range of arctan as \(0 \leq \arctan \phi < \pi\). \(\phi\) is the angle between the y axis and the line connecting the origin and \((x, y)\), so that \(x = r \sin \phi\) and \(y = r \cos \phi\). By using the transformed variables, the Hamiltonian in equation (8) are rewritten as \(H^{(3)} = H^{\text{HO}}(X; M_{e}, \omega_0) + H_{\text{rad}}(r, \phi)\), where

\[
H_{\text{rad}}(r, \phi) \equiv -\frac{1}{2m_r} \left[ \frac{\partial^2}{\partial r^2} + \frac{1}{r} \frac{\partial}{\partial r} - \frac{L(\phi)}{r^2} \right] + \frac{m_e \omega_0^2 \lambda_3^2}{2} r^2. \tag{14}
\]

\(L(\phi) \equiv -\partial^2 / \partial \phi^2, M_3 \equiv 3 m_e\), and \(\lambda_3 \equiv \sqrt{1 - 3 \lambda}\). For \(\lambda > 1/3\), such strong repulsive interactions do not allow the three electrons to form a bound state.

\(\phi(x_1, x_2, x_3) \equiv \phi(123)\) is anti-symmetric under the exchange of \(x_1\) and \(x_2\) (see equations (10)–(13)). In addition, as proved in appendix \(B\), \(\phi(123)\) and those with permuted \(x_1, x_2, x_3\) are related via the following relations:

\[
\phi(231) = \phi(123) + \frac{2\pi}{3}, \quad \phi(312) = \phi(123) + \frac{4\pi}{3}. \tag{15}
\]

2.3.2. Spatial wave functions. The Hamiltonian in equation (14) suggests the solution for the spatial WF of the form \(\Psi_{\alpha}(x_1, x_2, x_3) = \psi_{\alpha}^{\text{HO}}(\sqrt{3}X; \ell, \sqrt{3})R(r)\Phi_{\mu}^{\pm}(\phi)\), where \(\Phi_{\mu}^{\pm}(\phi) = \cos(m\phi)\sqrt{\frac{\Gamma}{\pi}}\) for \(m = 0, 1, \ldots\) and \(\Phi_{\mu}^{\pm}(\phi) = \sin(m\phi)\sqrt{\frac{\Gamma}{\pi}}\) for \(m = 1, 2, \ldots\). Substitution of this WF into the time-independent Schrödinger equation \(H^{(3)}\Psi_{\pm} = E^{(3)}\Psi_{\pm}\) with the Hamiltonian in equation (14) leads to the following eigenvalue equation that has to be satisfied by \(R(r)\):

\[
\left[ -\frac{1}{2m_r} \left( \frac{d^2}{dr^2} + \frac{1}{r} \frac{d}{dr} - \frac{m^2}{r^2} \right) - \frac{m_e \omega_0^2 \lambda_3^2}{2} r^2 \right] R(r) = E_r R(r). \tag{16}
\]

\(E_r \equiv E^{(3)} - E_{ck}\) and \(E_{ck} \equiv \omega_0(k + 1/2)\) is the contribution from the center-of-mass motion to the total energy. We assume the decaying solution of the form \(R(r) = r^\delta \exp(-r^2/2u(r)\delta)\) using the dimensionless coordinate \(\tau \equiv \sqrt{\lambda_3/2}(r/\ell)\) and substitute it into equation (16) to obtain the following equation:

\[
2\rho u \frac{d^2 u}{dr^2} + 2(m + 1 - \rho) \frac{du}{dr} + \left( \frac{E_r}{\lambda_3 \omega_0} - m - 1 \right) u = 0, \tag{17}
\]

where \(\rho \equiv r^2\). In order for \(u\) to be bounded when expressed in a series of \(\rho\), the series has to be truncated at some order \(n\). This condition leads to the eigenvalue as \(E_{\text{rms}} = \lambda_3 \omega_0(2n + m + 1)\). The solution of equation (17) for the eigenfunction \(u_{\text{rms}}\) belonging to \(E_{\text{rms}}\) is the associated Laguerre polynomial \(L^0_n(\rho)\), with which the solution of the radial equation in equation (16) is then

\[
R_{\text{rms}}(r) = \sqrt{\frac{2\nu}{(n + m)!} \frac{\lambda_3}{\ell} r^m e^{-r^2/2L^0_n(r^2)}, \tag{18}
\]

having the normalization constant for the condition in equation (A.2).

Gathering the solutions derived above, we obtain the expression for the explicitly correlated spatial WF

\[
\Psi_{\alpha,\text{rms}}(x_1, x_2, x_3) = \psi_{\alpha}^{\text{HO}}(\sqrt{3}X; \ell, \sqrt{3}) R_{\text{rms}}(r) \Phi_{\mu}^{\pm}(\phi), \tag{19}
\]

and its corresponding energy eigenvalue

\[
E_{\alpha,\text{rms}}^{(3)} = \omega_0 \left( k + \frac{1}{2} \right) + \lambda_3 \omega_0(2n + m + 1), \tag{20}
\]

characterized by the three quantum numbers. We should keep in mind that, at this point, neither the Fermi statistics nor the spin states have been taken into account.

2.3.3. Spin wave functions. Taut et al \[24\] constructed approximate three-electron WFs including spin parts for an interacting three-dimensional system for the perturbative analyses of correlation effects. The construction of eigenstates for two-spin states is straightforward, as widely instructed in textbooks of quantum mechanics and solid-state physics. The situation is, however, become complicated when there exist three spins in a target system. Taut et al provided the eigenstates of total spin of the three electrons explicitly by using the representation matrices of permutations. We adopt their manner for the construction of the three-electron WFs in the present study.

The following four linear combinations of the \(8 = 2^3 = 8\) bases for spin WFs form the spin quartet \((S = 3/2)\) states:

\[
\chi^{3/2, 3/2}(s_1, s_2, s_3) = \alpha(s_1)\alpha(s_2)\alpha(s_3). \tag{21}
\]
\[ \chi^{3/2,1/2}(s_1, s_2, s_3) = \frac{1}{\sqrt{3}} [\alpha(s_1)\alpha(s_2)\beta(s_3) + \alpha(s_1)\beta(s_2)\alpha(s_3) + \beta(s_1)\alpha(s_2)\alpha(s_3)] \tag{22} \]
\[ \chi^{3/2, -1/2}(s_1, s_2, s_3) = \frac{1}{\sqrt{3}} [\beta(s_1)\beta(s_2)\alpha(s_3) + \beta(s_1)\alpha(s_2)\beta(s_3) + \alpha(s_1)\beta(s_2)\beta(s_3)] \tag{23} \]
\[ \chi^{3/2, -3/2}(s_1, s_2, s_3) = \beta(s_1)\beta(s_2)\beta(s_3). \tag{24} \]

It is obvious that these spin WFs are symmetric under the exchange of an arbitrary two spin variables. When a spatial WF \( f(x_1, x_2, x_3) \equiv f(123) \) is given, one can easily construct the corresponding three-electron WF for \( S = 3/2 \) state as
\[ \begin{align*}
\chi^{3/2, 3/2}(x_1, x_2, x_3, s_1, s_2, s_3) &= \chi^{3/2, S}(s_1, s_2, s_3) A\phi(x_1, x_2, x_3), \tag{25} \\
\end{align*} \]
where the anti-symmetrization symbol \( A \) acts as
\[ A\phi(123) = \sum_{\sigma} \text{sgn}(\sigma) P_{\sigma} \phi(123) \]
\[ = f(123) - f(213) - f(132) + f(321) + f(231) + f(312). \tag{26} \]
\( \sigma \) is an element of the set \( \{1, 1, 2, 2, 3, 1, 3, 2, 1, 3, 2\} \) of permutations for \( \{1, 2, 3\} \) and \( P_{\sigma} \) is the corresponding operator for the three variables. The WF in equation (25) is clearly anti-symmetric under an arbitrary exchange of two electrons.

The remaining four spin bases form two doublets for spin singlet \( (S = 1/2) \) states:
\[ \chi_{1/2}^{1/2, 1/2}(s_1, s_2, s_3) = \frac{1}{\sqrt{6}} [-\alpha(s_1)\beta(s_2)\alpha(s_3) - \beta(s_1)\alpha(s_2)\alpha(s_3) + 2\alpha(s_1)\alpha(s_2)\alpha(s_3)] \tag{27} \]
\[ \chi_{1/2, -1/2}^{1/2}(s_1, s_2, s_3) = \frac{1}{\sqrt{6}} [\beta(s_1)\alpha(s_2)\beta(s_3) + \alpha(s_1)\beta(s_2)\beta(s_3) - 2\beta(s_1)\beta(s_2)\alpha(s_3)] \tag{28} \]
as the first one and
\[ \chi_{1/2}^{1/2, -1/2}(s_1, s_2, s_3) = \frac{1}{\sqrt{2}} [\alpha(s_1)\beta(s_2)\alpha(s_3) + \alpha(s_1)\beta(s_2)\alpha(s_3) - \beta(s_1)\alpha(s_2)\alpha(s_3)] \tag{29} \]
\[ \chi_{1/2}^{1/2, 1/2}(s_1, s_2, s_3) = \frac{1}{\sqrt{2}} [-\beta(s_1)\alpha(s_2)\beta(s_3) + \alpha(s_1)\beta(s_2)\beta(s_3) + \beta(s_1)\alpha(s_2)\beta(s_3) \tag{30} \]
as the second one. \( \chi_{1/2}^{1/2, S}(s_1, s_2, s_3) \) is symmetric (anti-symmetric) under the exchange of \( s_1 \) and \( s_2 \), whereas it is not symmetric (anti-symmetric) under the other exchanges. In fact, construction of a spin eigenstate of \( S^2 \) and \( S_z \) for three electrons that is symmetric or anti-symmetric under an arbitrary exchange is impossible. \( \chi_{1/2}^{1/2, S} \) and \( \chi_{1/2}^{1/2, S} \) for a given \( S \) are mixed with each other when a permutation operation is applied to the spin variables. Specifically, for a permutation \( \sigma \), the action of its corresponding operator to an \( S = 1/2 \) state is expressed as
\[ P_{\sigma} \chi_{j}^{1/2, S}(s_1, s_2, s_3) = \sum_{j' = 1,2} \chi_{j'}^{1/2, S}(s_1, s_2, s_3) (P_{\sigma})_{j'j} \tag{31} \]
for \( j = 1, 2 \) with the representation matrices \( P_{\sigma} \) [24]:
\[ P_{1} = \begin{pmatrix} 1 & 0 \\ 0 & 1 \end{pmatrix}, \quad P_{(1,2)} = \begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix} \]
\[ P_{(2,3)} = \begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix} \]
\[ P_{(1,2,3)} = \begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix} \]
and we used another arbitrary exchange of two electrons by using the fact that the permutations form a group of

2.3.4. Simultaneous eigenstates of energy and spin. We are now prepared to construct the simultaneous eigenstates of the energy, the total spin \( S \), and the \( z \) component \( S_z \) of total spin.

Since \( \phi(123) \) is anti-symmetric under the exchange of \( x_1 \) and \( x_2 \) as stated above, \( \Phi_{m}^{\sigma}(\phi(123)) \) vanishes when \( A \) is applied: \( A\Phi_{m}^{\sigma}(\phi(123)) = 0 \), indicating that an eigenstate for \( S = 3/2 \) cannot be constructed from the spatial WFs in equation (19) containing \( \Phi_{m}^{\sigma} \). On the other hand, the application of \( A \) to \( \Phi_{m}^{\sigma}(\phi(123)) \) can generate a non-vanishing function:
\[ A\Phi_{m}^{\sigma}(\phi(123)) = 2(\Phi_{m}^{\sigma}(\phi(231)) + \Phi_{m}^{\sigma}(\phi(312))) \]
\[ = 6\Phi_{m}^{\sigma}(\phi(123)) \quad (p = 0) \]
\[ = 0 \quad (p = 1, 2), \tag{34} \]
where we express \( m = 3m' + p \) with \( p = 0, 1, 2 \) and we used equation (15). We can thus construct the simultaneous eigenstate of the energy, \( S = 3/2 \), and \( S_z \) by using equation (25) for \( \Psi_{km}^{S} \) in equation (19) with \( p = 0 \) \( (m = 3, 6, 9, \ldots) \)
\[ \Psi_{km}^{S}(x_1, x_2, x_3) = \Psi_{km}^{S}(123) \chi_{m/2}^{S}(123). \tag{35} \]

For the construction of three-electron WFs for \( S = 1/2 \) states, we adopt equation (33) for \( \Psi_{km}^{S} \) by referring to the representation matrices in equation (32). The anti-symmetrized WFs from \( \Psi_{k1}^{S} \) for \( j = 1 \) and that from \( \Psi_{k2}^{-} \) for \( j = 2 \) vanish:
\[ \Psi_{k1}^{S, 1/2, 1+} = \Psi_{k2}^{S, 1/2, 2-} = 0. \]
On the other hand, the anti-symmetrized WF from \( \Psi_{k1}^{S} \) for \( j = 1 \) can be a non-vanishing function given by
We have constructed explicitly the simultaneous eigenstates of the energy and total spin of the three-electron system, as the first main result of the present study. The simultaneous eigenstates for a non-interacting case are provided in appendix C.

2.3.5. Energy spectra. Some of the lowest eigenvalues $E_{\mathrm{int}}^{(3)}$ in equation (20) and the corresponding three-electron WFs, the total spin, and the degeneracy are shown in table 1. The ground states are doubly degenerate $S = 1/2$ states, corresponding to $(k, n, m) = (0, 0, 1)$. The energy eigenvalues in table 1 as functions of $\Lambda$ are plotted in figure 1. The energy eigenvalues do not depend explicitly on the spin of the three-electron state since the system is time-reversal invariant.

By comparing the energy eigenvalues for the interacting case in table 1 and those for the non-interacting case in table C1, we find that the four-fold degenerate non-interacting states with $E_{\mathrm{int}}^{(3)}(0,0,1)/\omega_0 = 7/2$ split into the two doubly degenerate states when the interaction is turned on. We find similarly that the ten-fold degenerate non-interacting states with $E_{\mathrm{int}}^{(3)}(0,0,-1)/\omega_0 = 9/2$ split into the six-fold degenerate states and the two doubly degenerate states when the interaction is turned on. These observations corroborate our construction of the simultaneous eigenstates of the energy and total spin for the interacting system.

The electron density of the ground state for the three-electron system is now available since we know the exact WF, it will be interesting to compare the exact energy spectra and those calculated within DFT [25–30]. We did not adopt the so-called soft Coulomb interaction, which is often used in modeling one-dimensional systems [31], since we let the analytical solvability come first. If we resort to numerical solutions of the Schrödinger equation, the soft Coulomb interaction allows us to study more realistic models and to discuss the differences in WFs and GFs from the present model.

3. One-particle Green’s functions

3.1. Chemical potential and electron number

Since we consider the one-particle GF of the two-electron system at a zero temperature ($T = 0$), we have to take into account only the electron numbers up to 3. The expected electron number is thus given by $N_e = Z^{-1} \sum_{N=1}^{3} \sum_{\nu} N \exp \left[-(E_{\nu}^{(N)} - \mu)/k_B T\right]$, where $Z$ is the partition function and $\mu$ is the chemical potential. $\nu$ labels a many-body energy eigenstate for a fixed $N$. $N_e$ coincides with $N$ such that $E_{\nu}^{(N)} - \mu N$ is the lowest among all the possible $N$ and $\nu$ in the present case. To examine the allowed combinations of $\Lambda$ and $\mu$ for realization of $N_e = 2$, we define the following quantities from equations (3) and (20):

$$
\Delta^{(12)} \equiv (E_{0}^{(1)} - \mu) - (E_{00}^{(2)} - 2\mu) = -\frac{\lambda_2}{2} \omega_0 + \mu
$$

$$
\Delta^{(13)} \equiv (E_{0}^{(1)} - \mu) - (E_{00}^{(3)} - 3\mu) = -2\lambda_3 \omega_0 + 2\mu
$$
The behavior of $\Delta^{(12)}$, $\Delta^{(13)}$, and $\Delta^{(23)}$ as functions of $\Lambda$ and $\mu$. Only when the point $(\Lambda, \mu)$ is in the shaded region, $N_e = 2$. The three curves cross at $(\Lambda = 0.3, \mu = \omega_0/\sqrt{10})$.

\[
\Delta^{(23)} = (E_{00}^{(2)} - 2\mu) - (E_{01}^{(3)} - 3\mu) = \left(\frac{\lambda_2}{2} - 2\lambda_3\right)\omega_0 + \mu.
\]

(40)

The behavior of $\Delta^{(12)}$, $\Delta^{(13)}$, and $\Delta^{(23)}$ as functions of $\Lambda$ and $\mu$ are plotted in figure 2, indicating that $N_e = 2$ can be realized depending on the combination of the interaction strength and the chemical potential. The largest allowed value of the interaction strength is $\Lambda_{\text{max}} = 0.3$ for realization of $N_e = 2$, as found in the figure.

The one-, two-, and three-electron systems are equally stable at the critical point $(\Lambda = 0.3, \mu = \omega_0/\sqrt{10})$ in figure 2. Since the degeneracies of ground states for the $N$-electron systems $n_{gs}^{(N)}$ are $n_{gs}^{(1)} = 2$, $n_{gs}^{(2)} = 1$, and $n_{gs}^{(3)} = 2$, we can calculate easily the fluctuation of electron number at the critical point as $\delta N_e^2 = (N^2) - (N)^2 = 4/5$, which is interestingly nonzero despite the zero temperature.

We assume a combination of $\Lambda$ and $\mu$ for $N_e = 2$ in what follows.

3.2. Interacting Green’s functions

3.2.1. Spectral representation. Since the ground state of the two-electron system given in equation (7) is non-degenerate, the partition function is unity: $Z = 1$. The one-particle GF for a complex frequency $\omega$ is then written as

\[
\begin{align*}
\Delta^{(23)} & = \left(E_{00}^{(2)} - 2\mu\right) - \left(E_{01}^{(3)} - 3\mu\right) = \left(\frac{\lambda_2}{2} - 2\lambda_3\right)\omega_0 + \mu. \\
\end{align*}
\]

(40)

and

\[
G_{st}^{(e)}(x, x', z) = \sum_{\kappa} \frac{\langle \Psi_{st}^{(2)} | \hat{\psi}(x, s) | \Psi_{st}^{(2)} \rangle \langle \Psi_{st}^{(3)} | \hat{\psi}(x', s') | \Psi_{st}^{(2)} \rangle}{z + \mu + E_{gs}^{(1)} - E_{gs}^{(3)}}
\]

(43)

are the partial GFs [32] at a zero temperature for hole and electron excitations, respectively, in spectral representation. $\kappa$ in equations (42) and (43) runs over all the many-body energy eigenstates for a given electron number.

3.2.2. Hole excitation. For the spatial parts of the one- and two-electron WFs, we define the integral

\[
M_n(x_2) \equiv \int_{-\infty}^{\infty} dx_1 \hat{H}_n (\frac{x_1}{\ell})^* \Psi_{00}(x_1, x_2)
\]

\[
= \frac{m_0 \omega_0 \lambda_2}{\pi^3} \left\{ \begin{array}{ll}
\frac{1}{2} & \text{for } \nu = 0.5 \\
\frac{3}{2} & \text{for } \nu = 1 \\
\end{array} \right.
\]

(44)

where $\lambda_{\nu} \equiv x_2/\ell$ and equation (4) was used. With this, the matrix element of the annihilation operator (see equation (A.4)), often called the quasihole wave function, is written as

\[
\Psi_{00}^{(2)}(x_1, x_2, s_1, s_2) = \begin{cases}
M(x_2)\beta(s_2)/\sqrt{2} & (S_z = 1/2) \\
-M(x_2)\alpha(s_2)/\sqrt{2} & (S_z = -1/2)
\end{cases}
\]

(45)

Substitution of this into equation (42) and the completeness of spin WFs, $\alpha(s)\alpha(s')^* + \beta(s)\beta(s')^* = \delta_{ss'}$, lead to

\[
G_{st}^{(e)}(x, x', z) = \sum_{n=0}^{\infty} \delta_{st} \frac{M_n(x)}{z + \mu + (n - \lambda_2/2)\omega_0}
\]

(46)

where the spin-independent GF

\[
G^{(b)}(x, x', z) = \frac{1}{2} \sqrt{\frac{m_0^2\lambda_2}{\pi^3\omega_0}} \left(\frac{1}{\ell}\frac{x}{\ell}, \frac{x'}{\ell}, z\right) \left|_{\omega = (z + \mu)/\omega_0 - \lambda_2/2} \right.
\]

(47)

is calculated from the dimensionless quantity

\[
F^{(b)}(x, x', z) = \int_{-\infty}^{\infty} d\zeta K^+(\zeta, \pi, z) \int_{-\infty}^{\zeta} d\zeta' K^- (\zeta', x, z) + \int_{-\infty}^{\infty} d\zeta K^- (\zeta, \pi, z) \int_{-\infty}^{\zeta} d\zeta' K^+ (\zeta', x', z)
\]

(48)
with
\[
K^\pm(\zeta, x, z) \equiv \exp \left( -\frac{1 + \lambda_2}{8} \zeta^2 - \frac{1 - \lambda_2}{4} \zeta - \frac{1 + \lambda_2}{8} x^2 \right) D_{-\nu}(\pm \zeta). \tag{49}
\]

To get the expression in equation (49), we used the formula provided by Glasser and Nieto [33], which expresses the infinite summation over the Hermite polynomials via the parabolic cylinder function $D_\nu [34]$. The pole positions of $G^{(b)}$ on the $z$ axis are those of the Gamma function in equation (47), which are given by
\[
z + \mu - \frac{\lambda_2}{2} = 0, -1, -2, \ldots \tag{50}
\]
Each of these pole positions corresponds to a certain $n$ in equation (46), indicating that the pole for $n = 0$ represents a one-electron system where the electron occupies the lowest-energy orbital after the removal of an electron from the two-electron system. This process contributes as a major peak of the imaginary part of $G^{(b)}$ on the $z$ axis, known as a quasiparticle peak. The other processes ($n \neq 0$) represent the systems, in which of which the remaining electron is excited. They contribute as minor peaks known as satellite peaks. The obvious difference in the strength between these two kinds of peaks for hole excitations will be demonstrated later.

### 3.2.3. Electron excitation
Since the ground state of the two-electron system is $S = 0$, no transition to an $S = 3/2$ state occurs when an electron is added to the system:
\[
\langle \Psi_{k\mu m}^s | \hat{\psi}^\dagger(x, s) | \Psi_{gs}^{(2)} \rangle = 0 \ (p = 0). \tag{51}
\]

By using the integral
\[
M_{k\mu m}^\pm(x_3) \equiv \int dx_1 dx_2 \psi_{k\mu m}^\pm(x_1, x_2, x_3) \psi_{00}(x_1, x_2) \tag{52}
\]
for the spatial parts of the two- and three-electron WFs with $p = 1, 2$ and
\[
M_{j}^S(s_3) \equiv \sum_{s_1, s_2} \chi_j^{1/2} \chi_j^{s_1} \chi_0^{s_2} \tag{53}
\]
for the spin parts (see appendix D), the matrix element of the quasiparticle wave function, is written as
\[
\langle \Psi_{k\mu m}^s | \hat{\psi}^\dagger(x_3, s_3) | \Psi_{gs}^{(2)} \rangle = \frac{1}{2!} \sum_{s_1, s_2} \int dx_1 dx_2 \psi_{k\mu m}^\dagger(x_1, s_1, x_2, s_2, x_3) \psi_{gs}^{(2)}(x_1, s_1, x_2, s_2) = \pm \frac{1}{2\sqrt{2}} M_{j}^S(s_3) M_{k\mu m}^\pm(x_3), \tag{54}
\]
where the negative (positive) sign on the right-hand side is for $p = 1$ ($p = 2$). The explicit expression of $M_{k\mu m}^\pm(x_3)$ is derived in appendix E. Substitution of equation (54) into equation (43) and the completeness of spin WFs lead to
\[
G^{(e)}_{\nu \nu'}(x, x', z) = \delta_{\nu \nu'} \frac{1}{8} \sum_{k, n, m(p = 1, 2)} \frac{M_{k\nu m}^\dagger(x) M_{k\nu m}^\dagger(x')}{z + \mu - (k + d_{nm})\omega_0} \tag{55}
\]
where $\omega_0$ is a small deviation of $\delta$ from the poles on the real axis.

![Figure 3. Imaginary part of integrated partial GF $G^{(b)}$ near its three poles closest to the origin of $z$ as function of the interaction strength. $\delta$ is a small deviation of $\delta$ from the poles on the real axis.](image)

\[
F^{(e)}_{\nu \nu'}(x, x', z) = -4 \sqrt{\frac{\lambda_2}{\pi \omega_0}} \sum_{n, m(p = 1, 2)} \frac{1}{n!} \Gamma(\nu_{nm}) \tag{56}
\]
is calculated from the dimensionless quantity
\[
F^{(e)}_{\nu \nu'}(x, x', z) = \int_{-\infty}^{\infty} d\zeta K^{+\dagger}_{\nu_{nm}}(\zeta, x, z) \int_{-\infty}^{\infty} d\zeta' K_{\nu_{nm}}(\zeta', x', z) \tag{57}
\]
with
\[
K_{\nu_{nm}}(\zeta, x, z) \equiv \exp \left[ -\frac{(\zeta + x)^2}{2} \right] D_{-\nu_{nm}}(\pm \frac{\sqrt{\lambda_2}}{\sqrt{x + \zeta}}) \tag{58}
\]
for which $I_{\nu_{nm}}$ is defined in equation (E.8). To get the expression in equation (58), we used the formula [33] for the infinite summation over the Hermite polynomials. The pole positions of $G^{(b)}$ on the $z$ axis are those of the Gamma function in equation (56), which are given by
Each of these pole positions corresponds to a certain $k$ in equation (55) for given $n$ and $m$, indicating that a pole for $k = 0$ ($k \neq 0$) represents a three-electron system where the center-of-mass motion is not excited (is excited) after the addition of an electron to the two-electron system.

We have obtained finally the exact expressions of the GF for the two-electron system, as the second main result of the present study. The expressions for the partial GFs we derived are more favorable than the generic expressions in equations (42) and (43) for practical calculations. It is because the summation over one of the three quantum numbers has been already taken exactly in our expressions.

3.3.4. Pole strengths. Photoemission spectra [11–13] are related to the one-particle GF integrated over spatial variable in general. Here we examine the integrated GF of our system

$$G(z) = \int_{-\infty}^{\infty} dx G(x, x, z),$$

(60)

for which we plot the imaginary part of $G^{(b)}(z)$ near the poles in figure 3. It is seen that the magnitudes near the first pole, which is identified as the quasiparticle peak at $z + \mu = \lambda_2/2$ (see equation (59)), is much larger than those near the other poles, identified as the satellite peaks. These observations indicate that the independent-particle picture is basically valid for the hole excitation process, realizing the quasiparticle peak, while the many-electron effects cause the satellite peaks.

3.3. Non-interacting Green’s functions

It is instructive to compare the interacting GFs and the corresponding (non-interacting) KS GFs. We derive the expressions for the latter ones here.

3.3.1. Hole excitation. When the interaction is absent ($\Lambda = 0$), the integral $M_n(x_2)$ in equation (44) is nonzero only for $n = 0$. The spin-independent partial GF for hole excitations are then calculated as

$$G^{(b)\text{non-int}}(x, x', z) = \sqrt{\frac{m_e}{\pi \omega_0}} \exp\left[-z^{2}/\omega_0 \right]$$

(61)

where $x \equiv x/\ell$ and $x' \equiv x'/\ell$, as a special case of equation (47).

3.3.2. Electron excitation. For the derivation of expressions for the non-interacting GF for electron excitations, it is easier to work with the quantum numbers $(n_1, n_2, n_3)$ for the independent oscillators described in appendix C than those for the interacting case, $(k, n, m)$.

Since the ground state of the non-interacting two-electron system consists of two electrons occupying the lowest-energy spatial orbital to form an $S = 0$ state, the normalized WF is given by $\psi_{1/2S_n}^{0}(x_1, x_2, s_1, s_2) = \sqrt{2} \psi_0(x_1) \psi_0(x_2) \chi_{00}^{0}(s_1, s_2)$. When an electron is added to the system, the electron occupies another spatial orbital $\psi_n$ with $n \neq 0$ to form a three-electron system whose WF is given by $\psi_{1/2S_n}^{0}$ in equation (C.2). The matrix element of the creation operator is then calculated as (see appendix D)

$$\langle \psi_{1/2S_n}^{0}\mid \hat{\alpha}(s_1)\hat{\beta}(s_2)\mid \psi_{1/2S_n}^{0}\rangle = \psi_n^{*}(s_1)\chi_{s_2}^{0}$$

(62)

which is then substituted into equation (43) to get the spin-independent partial GF for electron excitations:

$$G^{(e)\text{non-int}}(x, x', z) = -\sum_{n=1}^{\infty} \frac{\psi_n(x)\psi_n(x')^*}{\omega_0}$$

$$= \sqrt{\frac{m_e}{\pi \omega_0}} \exp\left(-\frac{z^2}{2}\right)$$

$$-\Gamma(\nu)D_{\nu}(\xi_\sigma)D_{\nu}(\xi_\pi)$$

(63)

$\xi_\sigma$ and $\xi_\pi$ are defined for $\xi$ and $\xi'$ so that $\xi_\sigma > \xi_\pi$. To get the last equality in equation (63), we used the formula for the infinite summation over the Hermite polynomials provided by Glasser and Nieto [33], who derived the expression of the non-interacting GF, $G^{\text{non-int}} = G^{(b)\text{non-int}} + G^{(e)\text{non-int}}$.

3.3.3. Kohn–Sham Green’s function. It is well known that the exact KS potential for ground state of an interacting two-electron system can be constructed if the electron density $n_{\text{gs}}^{(2)}(r)$ of the spin-singlet ground state is known [31, 35, 36]:

$$V_{\text{KS}}(r) = \frac{\nabla^2 n_{\text{gs}}^{(2)}(r)}{2m_e n_{\text{gs}}^{(2)}(r)}$$

(64)

The exact KS potential for our interacting two-electron system is calculated from equations (7) and (64) as [22]
It is clear that this KS Hamiltonian for the effective non-interacting system is obtained apart from a constant simply by replacing \( \omega_0 \) with \( 2\omega_0\lambda_2/(1 + \lambda_2) \equiv \varepsilon_{\text{KS}}^2\omega_0 \) and setting \( \Lambda = 0 \) in the original Hamiltonian in equation (1). The \( n \)-th KS orbital energy is thus given by

\[
\varepsilon_n^{\text{KS}} = \varepsilon_{\text{KS}}^2\omega_0 \left(n + \frac{1}{2}\right).
\]

With the positive constant \( \varepsilon_{\text{KS}} \), the partial GFs of the KS system are obtained via the replacement for equations (61) and (63) as

\[
G^{(b)\text{KS}}(x, x', z) = -\sqrt{\frac{m_e}{\pi\omega_0}} \frac{1}{\alpha_{\text{KS}}} \exp[-\alpha_{\text{KS}}^2(x^2 + x'^2)/4] \left(\frac{\nu_{\text{KS}}}{\nu_{\text{KS}} - \mu}\right) \left(e^{\nu_{\text{KS}}\lambda} - e^{-\nu_{\text{KS}}\lambda}\right)
\]

and

\[
G^{(e)\text{KS}}(x, x', z) = -\sqrt{\frac{m_e}{\pi\omega_0}} \frac{1}{\alpha_{\text{KS}}} \exp[-\alpha_{\text{KS}}^2(x^2 + x'^2)/4] \left(\frac{\nu_{\text{KS}}}{\nu_{\text{KS}} + \mu}\right) \left(e^{-\nu_{\text{KS}}\lambda} - e^{\nu_{\text{KS}}\lambda}\right),
\]

where \( \nu_{\text{KS}} = -(\mu + z)/(\alpha_{\text{KS}}\omega_0) + 1/2 \). We have adopted the chemical potential of the original system as that for the KS system.

The pole positions of \( G \) and those of \( G^{\text{KS}} \) on the energy axis (real axis of \( z \)) as functions of \( \Lambda \) are plotted in figure 4. One finds that there exist more non-degenerate poles for an interacting \( \Lambda \neq 0 \) case than in the corresponding KS system.

Furthermore, the discrepancies between the pole positions of \( G \) and those of \( G^{\text{KS}} \) become larger as the interaction becomes stronger. There exists only one pole coming from \( G^{(b)\text{KS}} \), while an infinite number of poles from \( G^{(b)} \) exist in the negative direction of \( z \) axis. For both of \( G^{(e)} \) and \( G^{(e)\text{KS}} \), on the other hand, there exist an infinite number of poles in the positive \( z \) direction.

The fundamental gap is calculated as \( E_{\text{gap}} = E_{\text{KS}}^{(3)} - 2E_{\text{KS}}^{(2)} + E_{\text{KS}}^{(1)} = \omega_0(2\lambda_2 - \lambda_1) \), while the HOMO-LUMO gap of the KS system is \( E_{\text{gap}}^{\text{KS}} = \varepsilon_1^{\text{KS}} - \varepsilon_0^{\text{KS}} = 2\omega_0\lambda_2/(1 + \lambda_2) \). One can easily confirm that \( E_{\text{gap}} < E_{\text{gap}}^{\text{KS}} \) for the allowed range of \( \Lambda \). This fact is also understood by looking at figure 4, where \( E_{\text{gap}} \) (\( E_{\text{gap}}^{\text{KS}} \)) is nothing but the distance between the neighboring poles on the \( z \) axis coming from \( G^{(b)} \) and \( G^{(e)} \) (\( G^{(b)\text{KS}} \) and \( G^{(e)\text{KS}} \)). These observations indicate that our system is an example where even the exact KS potential does not give the correct energy gap particularly for strong interactions.

We can also calculate the pole positions of the exact GF of the three-electron system for hole excitation. (See appendix F)

![Figure 5](image)

**Figure 5.** Spin independent partial GFs for electron excitation. \( G^{(e)} \) with \( \Lambda = 0 \) using the expression for the interacting GF and \( G^{(e)\text{non-int}} \) as functions of \( x \) are plotted for (a) \( x'/\ell = 0, (z + \mu)/\omega_0 = 0 \) and (b) \( x'/\ell = 1, (z + \mu)/\omega_0 = 2 \). For the expression of \( G^{(e)} \), the GF for different truncations in infinite summations are plotted.

at some values \( n_{\text{max}} \) and \( m_{\text{max}} \) for a practical calculation. We first examined the convergence of \( G^{(e)} \) with respect to \( n_{\text{max}} \) and \( m_{\text{max}} \). \( G^{(e)} \) with \( \Lambda = 0 \) using equation (55) and \( G^{(e)\text{non-int}} \) using equation (63) as functions of \( x \) are plotted in figure 5. It is seen that \( G^{(e)\text{non-int}} \) has cusps at \( x = x' \). These features are not seen in the calculated \( G^{(e)} \) since, in general, the summation over a finite number of smooth functions gives another smooth function. It is also found, however, that the calculated \( G^{(e)} \) for larger \( n_{\text{max}} \) and \( m_{\text{max}} \) has more similar shapes to \( G^{(e)\text{non-int}} \). The convergence is slower for \( x \) near the cusps than for that away the cusps. We adopt \( n_{\text{max}} = m_{\text{max}} = 10 \) in what follows because this truncation leads to the satisfactory convergence for qualitative discussion in the present study.

The spin independent partial GFs as functions of \( x \) with fixed \( x' \) and \( z \) for \( \Lambda = 0.1 \) and 0.25 are plotted in figures 6 and 7, respectively. It is seen that the contributions from hole excitations are small compared to those from electron excitations both in the exact and the KS GFs. The shapes of the exact and KS GFs can change drastically as \( z \) crosses the poles on the frequency axis (see figure 4). More importantly, one finds that the shape and/or the magnitude of \( G^{(e)} \) for a given combination of \( x' \) and \( z \) are not similar to those of the corresponding

3.4. Numerical examination

Our expression of the interacting GF for electron excitations in equation (55) involves the infinite summation over the two quantum numbers. We have to truncate the summation
This observation reminds us of the fact that the foundation of DFT ensures only the correctness of the total energy and the electron density for the ground state of a given electronic system. In spite of this fact, the quantitative predictions provided by GF-based approach in electronic-structure calculations have been successful by and large. It is at least partially because the physical quantities to be predicted are calculated only via integration of the interacting GF of a realistic target system. The examination on the GFs of our model system provides us a lesson that we have to be careful if we want to know the shape of the GF itself using the DFT results as a reference state.

4. Conclusions

For a three-electron system with finite-strength interactions confined to a one-dimensional harmonic trap, we solved the Schrödinger equation analytically to obtain the exact solutions, from which we constructed explicitly the simultaneous eigenstates of the energy and the total spin for the first time.
The solutions for the three-electron system allowed us to derive the analytic expressions for the exact one-particle GF for the corresponding interacting two-electron system. We also derived the KS GF by using the exact KS potential for the two-electron system. We identified the pole positions of the exact and KS GFs and found that the discrepancies between them becomes larger for a stronger interaction.

We performed numerical examination on the behavior of GFs in real space. It was demonstrated that the exact and KS GFs can have shapes quite different from each other depending on the frequency and they can change drastically when the frequency crosses the poles, implying that careful analyses are required when a GF itself is examined within a mean-field-based approach.

We have now the exact solutions for the three-electron system at hand, it is possible to examine the many-body effects in the three-electron system without resorting to second-quantized form. It will be interesting to look for many-body effects in the three-electron system which are absent in the two-electron system. In addition, the two-electron system we considered will serve as a minimal real-space model having a non-trivial interacting GF. We expect that this simple model will help to find and understand generic characteristics of GFs.

Our prescription for the construction of eigenstates for three electrons is applicable for three bosons by paying attention to the Bose statistics. It is thus expected that the three-boson system equipped with the Schrödinger equation in the same form as in the present study will serve as a new analytically solvable model of interacting three bosons [37–39]. It is worth examining the exact GF of an interacting two-boson system.

Acknowledgments

This research was supported by MEXT as Exploratory Challenge on Post-K computer (Frontiers of Basic Science: Challenging the Limits). This research used computational resources of the K computer provided by the RIKEN Advanced Institute for Computational Science through the HPCI System Research project (Project ID: hp180227).

Appendix A. Many-electron wave functions

The normalization conditions and the definitions of matrix elements involving many-electron WFs are the same as in [40]. In order for this paper to be self-contained, we summarize the expressions necessary for the present study briefly here.

The completeness of the eigenstates of positions and spins for \(N\)-electron systems is expressed as

\[
\frac{1}{N!} \int d\xi_1 \cdots d\xi_N |\Psi^{(N)}(\xi_1, \ldots, \xi_N)\rangle^2 = 1, \tag{A.1}
\]

where \(\xi\) represents the position and spin variables collectively. For an \(N\)-electron state \(|\Psi^{(N)}\rangle\) normalized to unity \((\langle \Psi^{(N)} | \Psi^{(N)} \rangle = 1)\), the completeness in equation (A.1) imposes the normalization condition on the many-electron WF as

\[
\int d\xi_1 \cdots d\xi_N |\Psi^{(N)}(\xi_1, \ldots, \xi_N)\rangle^2 = N!. \tag{A.2}
\]

The electron density corresponding to a many-electron WF is calculated as

\[
n(\xi) = \frac{1}{(N-1)!} \int d\xi \cdots d\xi_{N-1} |\Psi^{(N)}(\xi_1, \ldots, \xi_{N-1}, \xi)\rangle^2, \tag{A.3}
\]

which gives, as expected, the total electron number: \(\int d\xi n(\xi) = N\).

By referring to the action of the creation operator of the electron field [40], we can express the matrix element of the operator as

\[
\langle \Psi^{(N+1)} | \hat{\psi}^\dagger(\xi) | \Psi^{(N)} \rangle = \frac{1}{N!} \int d\xi_1 \cdots d\xi_N \cdot \Psi^{(N+1)}(\xi_1, \ldots, \xi_N, \xi) \Psi^{(N)}(\xi_1, \ldots, \xi_N). \tag{A.4}
\]

The expression for the annihilation operator can be obtained by taking the complex conjugate of equation (A.4).

Appendix B. Proof of equation (15)

From equations (9)–(11), we have

\[
\begin{align*}
x_1 - x_2 &= \sqrt{2} r \sin \phi \\
x_2 - x_3 &= \sqrt{2} r \sin \left(\phi + \frac{2\pi}{3}\right) \\
x_3 - x_1 &= \sqrt{2} r \sin \left(\phi + \frac{4\pi}{3}\right).
\end{align*} \tag{B.1}
\]

The angle variable \(\phi(x_1, x_2, x_3) \equiv \phi(123)\) falls within the following ranges according to \(x_1, x_2\), and \(x_3\) (see equation (3.8) in [23]):

\[
\begin{aligned}
0 &< \phi(123) < \frac{\pi}{3} & (x_1 > x_2 > x_3) \\
\frac{\pi}{3} &< \phi(123) < 2\frac{\pi}{3} & (x_1 < x_3 < x_2) \\
2\frac{\pi}{3} &< \phi(123) < \pi & (x_3 > x_1 > x_2) \\
\pi &< \phi(123) < 4\frac{\pi}{3} & (x_3 > x_2 > x_1) \\
4\frac{\pi}{3} &< \phi(123) < 5\frac{\pi}{3} & (x_2 > x_3 > x_1) \\
5\frac{\pi}{3} &< \phi(123) < 2\pi & (x_2 > x_1 > x_3).
\end{aligned} \tag{B.2}
\]

The ranges of \(\phi(231)\) and \(\phi(312)\) are restricted similarly.

From equation (B.1), we obtain the relations between \(\phi(123)\), \(\phi(231)\), and \(\phi(312)\) as

\[
\tan \phi(231) = \frac{\sqrt{3}(x_2 - x_1)}{x_2 + x_3 - 2x_1} = \tan \left[\phi(123) + \frac{2\pi}{3}\right] \tag{B.3}
\]

and

\[
\tan \phi(312) = \frac{\sqrt{3}(x_3 - x_1)}{x_3 + x_1 - 2x_2} = \tan \left[\phi(123) + \frac{4\pi}{3}\right]. \tag{B.4}
\]

With these relations and equation (B.2), the three angle variables are found to satisfy equation (15).
Appendix C. Non-interacting case for three electrons

For a non-interacting case ($\Lambda = 0$), the spatial dynamics of the three-electron systems is described as that of three independent harmonic oscillators. The energy eigenvalue of the whole system is thus given by $E_{(n_1, n_2, n_3)}^{(3) non-int} = \omega_0 (n_1 + n_2 + n_3 + 3/2)$, where $n_1$, $n_2$, and $n_3$ are the quantum numbers for the independent oscillators. Since the three electrons are equivalent, it is clear that the electronic properties of the system are determined not by the order of the quantum numbers, but by the combination of them.

C.1. $n_1 = n_2 = n_3$ case

Any electronic configuration in which the three quantum numbers are equal to each other is impossible due to the Fermi statistics.

C.2. $n_1 \neq n_2 = n_3$ case

For $n_1 \equiv n \neq n_2 \equiv n' \neq n''$, the spatial WF $\psi_{n'n''}(x_1, x_2, x_3) \equiv \psi_n(x_1)\psi_n(x_2)\psi_{n''}(x_3)$ vanishes when it is anti-symmetrized: $\mathbf{F}\psi_{n'n''}(x_1, x_2, x_3) = 0$, indicating that the construction of an $S = 3/2$ state from this spatial WF is impossible (see equation (25)). On the other hand, by using equation (33) with $j = 1$, we can construct the anti-symmetrized three-electron WF for an $S = 1/2$ state as

$$\psi^{1/2, S, 1}_{n'n''}(x_1, x_2, x_3) = \sqrt{\frac{3}{2}} \chi_2^{1/2, S}(123)[\psi_{n'n''}(123) - \psi_{n'n''}(231)]$$

$$+ \frac{1}{\sqrt{2}} \chi_2^{1/2, S}(123)[\psi_{n'n''}(123) - \psi_{n'n''}(231) + 2\psi_{n'n''}(312)],$$

(C.1)

where we introduced a normalization constant. Although the anti-symmetrized WF $\psi^{1/2, S, 2}_{n'n''}$ from $\psi_{n'n''}$ for $j = 2$ can be constructed as well, one can confirm that it is the same WF as $\psi^{1/2, S, 1}_{n'n''}$. The simultaneous eigenstates of the energy, $S = 1/2$, and $S_z$ are thus covered by $\psi^{1/2, S, 1}_{n'n''}$:

$$\psi^{1/2, S, 1}_{n'n''}(x_1, x_2, x_3, x_4, x_5) \equiv \psi^{1/2, S, 1}_{n'n''}(x_1, x_2, x_3, x_4, x_5),$$

(C.2)

implying that the energy eigenstates for the combination $\{n, n', n''\}$ of quantum numbers are doubly degenerate.

C.3. $n_1 \neq n_2, n_2 \neq n_3, n_3 \neq n_1$ case

By using equation (25) for the spatial function $\psi_{n_1n_2n_3}(x_1, x_2, x_3) \equiv \psi_{n_1}(x_1)\psi_{n_2}(x_2)\psi_{n_3}(x_3)$, we can construct the anti-symmetrized three-electron WF for an $S = 3/2$ state as

$$\psi^{3/2, S}_{n_1n_2n_3}(123) = \chi^{3/2, S}(123)[\psi_{n_1n_2n_3}(123) - \psi_{n_1n_2n_3}(213) - \psi_{n_1n_2n_3}(132)$$

$$- \psi_{n_1n_2n_3}(321) + \psi_{n_1n_2n_3}(231) + \psi_{n_1n_2n_3}(312)].$$

(C.3)

Table C1. Some of the lowest eigenvalues $E^{(3) non-int}_{n_1n_2n_3}$ of the non-interacting three-electron system. The three-electron wave functions, the total spin $S$, and the degeneracy are also shown.

| $E^{(3) non-int}_{n_1n_2n_3}$ / $\omega_0$ | $\psi^{S, S}_{n_1n_2n_3}$ | degeneracy |
|------------------------------------------|--------------------------|-----------|
| 5/2                                      | $\psi^{1/2, S}_{100}$    | 2         |
| 7/2                                      | $\psi^{1/2, S}_{100}$    | 2         |
| 9/2                                      | $\psi^{1/2, S}_{210}$    | 4         |

By using equation (33) with $j = 1, 2$, we can construct the anti-symmetrized three-electron WF for $S = 1/2$ states:

$$\psi^{1/2, S, 1}_{n_1n_2n_3}(123) = \frac{1}{\sqrt{2}} \chi^{1/2, S}(123)[2\psi_{n_1n_2n_3}(123) - 2\psi_{n_1n_2n_3}(213) + \psi_{n_1n_2n_3}(132)$$

$$+ \psi_{n_1n_2n_3}(321) - \psi_{n_1n_2n_3}(231) - \psi_{n_1n_2n_3}(312)]$$

$$+ \frac{\sqrt{3}}{2} \chi^{1/2, S}(123)[\psi_{n_1n_2n_3}(132) + \psi_{n_1n_2n_3}(321) - \psi_{n_1n_2n_3}(231)].$$

(C.4)

and

$$\psi^{1/2, S, 2}_{n_1n_2n_3}(123) = \frac{\sqrt{3}}{2} \chi^{1/2, S}(123)[\psi_{n_1n_2n_3}(132) + \psi_{n_1n_2n_3}(321)]$$

$$+ \psi_{n_1n_2n_3}(231) - \psi_{n_1n_2n_3}(312) + \psi_{n_1n_2n_3}(123)$$

$$+ \frac{1}{2} \chi^{1/2, S}(123)[2\psi_{n_1n_2n_3}(123) + 2\psi_{n_1n_2n_3}(213)$$

$$- \psi_{n_1n_2n_3}(132) - \psi_{n_1n_2n_3}(321) - \psi_{n_1n_2n_3}(231) - \psi_{n_1n_2n_3}(312)],$$

(C.5)

which are easily confirmed to be orthogonal to each other. The energy eigenstates for the combination $\{n_1, n_2, n_3\}$ of quantum numbers are eight-fold degenerate.

Some of the lowest energy eigenvalues and the corresponding three-electron WFs, the total spin, and the degeneracy are shown in table C1. The ground states are doubly degenerate $S = 1/2$ states, corresponding to $\{n_1, n_2, n_3\} = \{1, 0, 0\}$.

Appendix D. Calculation of $M^S_j(s_3)$

The spin WF of a singlet state for two spins is given by $\chi^{0,0}(s_1, s_2) = [\alpha(s_1)\beta(s_2) - \beta(s_1)\alpha(s_2)]/\sqrt{2}$. By substituting this expression and equations (27) and (28) into equation (53) for $j = 1$ and using the orthonormality of the spin WFs, we can calculate the integrals as $M^{1/2}_1(s_3) = M^{1/2}_1(s_3) = 0$. We can also calculate those for $j = 2$ from equations (29) and (30) as $M^{1/2}_2(s_3) = \alpha(s_3)^* \alpha(s_3)$ and $M^{1/2}_2(s_3) = -\beta(s_3)^* \alpha(s_3)^*$. 


Appendix E. Calculation of $M_{kmn}^+(x_3)$

By substituting the expressions for the many-electron WFs in equations (4) and (19) into the definition equation (52) of the integral, we obtain

$$M^+_{kmn}(x_3) = \frac{m_{\omega,\lambda_0}}{\pi} 4\lambda_2^{1/4} \int dx_1 dx_2 \psi_k^{\text{HO}} \left( \frac{2x_1 + x_3}{\sqrt{3\ell}} ; \ell \right)$$

$$R_{\text{am}}(r) \Phi_m^+ (\phi) \exp \left[ -m_{\omega,\lambda_0} \left( x_1^2 + \frac{\lambda_2 x_1^2}{2} \right) \right].$$

(E.1)

To proceed the calculation, we consider the transformation of the integral variables from $(x_1, x_2)$ to $(x_+ r, r)$. It is confirmed that from equations (10)–(12) that $r, x_+$, and $x_-$ are related via the relation

$$r^2 = x_+^2 + \frac{2}{3}(x_+ - x_-)^2,$$

(E.2)

which represents an ellipse centered at $(x_3, 0)$ on the $x_+ - x_-$ plane for a given $r$. $x_1$ and $x_2$ are expressed in $x_+$ and $x_-$ as

$$x_1 = x_+ + x_- / \sqrt{2} \text{ and } x_2 = x_+ - x_- / \sqrt{2},$$

respectively. Since the integrand in equation (E.1) is invariant under the exchange of $x_1$ and $x_2$, it is necessary to consider only the case with $x_1 > x_2$, in which we can express $x_1$ and $x_2$ as functions of $x_+$ and $r$ as

$$x_{1,2} = x_+ \pm \sqrt{\frac{r^2}{2} - \frac{(x_+ - x_-)^2}{3}}.$$  

(E.3)

The positive (negative) sign on the right-hand side is for $x_1 (x_2)$. The Jacobian for the transformation of integral variables is then calculated as

$$\frac{\partial(x_1, x_2)}{\partial(x_+, r)} = \left[ 1 \pm \frac{(x_+ - x_-)^2}{3r^2} \right]^{-1/2}.$$  

(E.4)

For a given $x_+$, it is clear from equation (E.2) that the range of $r$ is $\sqrt{\frac{2}{3}} |x_+ - x_-| < r < \infty$ to represent $0 < x_- < \infty$. The integral measure in equation (E.1) is rewritten via the transformation as

$$\int dx_1 dx_2 = 2 \int_{x_+ > x_-} dx_1 dx_2$$

$$= 2 \int_{-\infty}^{\infty} dx_+ \int_{\sqrt{\frac{2}{3}} |x_+ - x_-|}^{\infty} dr \left| \frac{\partial(x_1, x_2)}{\partial(x_+, r)} \right|,$$

(E.5)

for which the coordinate systems are shown in figure E1. By using the transformation and introducing the dimensionless coordinates $\bar{x}_+ \equiv \sqrt{3}(x_+ - x_-)/\ell$ and $\bar{x}_- \equiv \sqrt{3}x_-/\ell$, we can rewrite equation (E.1) as

$$M^+_{kmn}(x_3) = \left( \frac{2\pi}{3} \right)^{1/4} \sqrt{\frac{32m!}{(n+m)!}} \int_{\bar{x}+1/3}^{\infty} d\bar{x}_+ \psi_k^{\text{HO}}$$

$$\left[ \frac{2}{3} \bar{x}_+ + \bar{x}_-, \ell \right] \exp \left[ \frac{(\bar{x}_+ + \bar{x}_-)^2}{6} + \frac{\lambda_2 \bar{x}_+^2}{18} \right].$$

$$\int_{\sqrt{\frac{2}{3}}|\bar{x}_+ - \bar{x}_-|}^{\infty} dr \frac{r_+^{m+1}}{\sqrt{1 - \lambda_2 \bar{x}_+^2/(9\ell^2)}} \exp \left[ -\frac{r_+^2}{2} \left( 1 + \frac{\lambda_2}{\bar{x}_+^2} \right) \right].$$

$$= \left( \frac{m_{\omega,\lambda_0}}{\pi^5} \right)^{1/4} \sqrt{\frac{32m!}{24k!(n+m)!}} \tilde{M}_{kmn}(x_3),$$

(E.6)

Figure E1. For a given $r$, allowed $x_+$ and $x_-$ form an ellipse centered at $(x_3, 0)$ on the $x_+ - x_-$ plane. For the integral over the region of $x_1 > x_2$, shaded in the figure, the range of integration variable $r$ for a fixed $x_3$ is $\sqrt{\frac{2}{3}} |x_+ - x_-| < r < \infty$.

Figure F1. Pole positions of the interacting GF of the three-electron system for hole excitation as functions of the interaction strength $\Lambda$. The quasiparticle peaks (QPs) and the satellite peaks (SPs) are distinguished in the plot for the transitions from the three-electron ground states (GSs) to the two-electron states.

where we used the expression of $R_{\text{am}}(r)$ in equation (18) and used the relation $\cos \phi = y/r = \bar{x}_+ \sqrt{\bar{x}_+/3}/(3\bar{r})$. We defined the dimensionless integral

$$\tilde{M}_{kmn}(\bar{x}) = \int_{-\infty}^{\infty} d\zeta \exp \left[ \frac{-1}{4} \frac{2}{3} \bar{x}^2 + \frac{\zeta^2}{\bar{x}_+^2} \right]$$

$$H_k \left( \frac{1}{\sqrt{2}} \left( \frac{2}{3} \zeta + \bar{x}_+ \right) \right) I_{km} \left( \frac{\sqrt{\bar{x}_+^2}}{3\zeta} \right),$$

(E.7)

with

$$I_{km}(\bar{r}_0) \equiv \int_{[\bar{r}_0]} d\bar{r} \frac{\bar{r}_m^{m+1}}{\sqrt{1 - \bar{r}_m^{2}/(\bar{r}_0^2)}} T_m^{(m)}(\bar{r})$$

$$T_m \left( \frac{\bar{r}_0}{\bar{r}} \right) \exp \left[ \frac{\bar{r}^2}{2} - \frac{\lambda_2}{2\lambda_3} (\bar{r}^2 - \bar{r}_0^2) \right]$$

$$= \left( \frac{\bar{r}_0^2}{\bar{r}^2} \right)^{m+1} \int_{[\bar{r}_0]} d\bar{r} \sqrt{\bar{r}_m^2 - 1} \frac{d}{d\zeta} \left[ \zeta^n L_n^m(\bar{r}_0^2\zeta^2) \right]$$

$$T_m \left( \frac{\bar{r}_0}{\bar{r}} \right) \exp \left[ \frac{\bar{r}_0^2}{2} - \frac{\lambda_2}{2\lambda_3} (\bar{r}^2 - \bar{r}_0^2) \right],$$

(E.8)

where we used partial integration. $T_m$ is the Chebyshev polynomial of the first kind, defined so that $T_m(\cos \phi) = \cos(m\phi).$
Appendix F. Hole excitation of three-electron system

Since we have the exact WFs for the two- and three-electron systems in hand, we can derive the analytic expressions for the interacting GF of the three-electron system for hole excitation. Here we discuss briefly their pole positions and the relation with the spectral intensities.

By using the WFs in equations (5) and (6) for the two-electron system, we can calculate the partial GFs $G^{(h)\rightarrow\text{singlet}}$ and $G^{(h)\rightarrow\text{triplet}}$ for the transitions from the three-electron ground states to the spin singlet and triplet two-electron states, respectively. Specifically, the spectral representations of $G^{(h)\rightarrow\text{singlet}}$ and $G^{(h)\rightarrow\text{triplet}}$ involve the infinite summation over even and odd $n_z$, respectively, while each of them involves that over all non-negative integers for $n_c$. We can thus use the formula [33] for the summation over $n_c$ to express $G^{(h)\rightarrow\text{singlet}}$ and $G^{(h)\rightarrow\text{triplet}}$ using the parabolic cylinder functions similarly to the GF of the two-electron system. One can easily find their expressions contain the Gamma functions whose poles are given by

$$\frac{z + \mu}{\omega_0} - 2\lambda_3 + \lambda_2 \left( n_z + \frac{1}{2} \right) = 0, -1, -2, \ldots$$  \hspace{1cm} (F.1)

which are nothing but the poles of $G^{(h)}$. The pole positions as functions of the interaction strength is plotted in figure F1. By comparing the two-electron WFs and the one-electron orbitals, it is found that the highest pole on $z$ axis corresponds to the HOMO for the unpaired electron in the three-electron system and the second and third highest ones correspond to the occupied lowest-energy orbitals. These three poles should thus be identified as the quasiparticle peaks in the spectral function. The other poles do not have corresponding one-electron orbitals and they are identified as the satellite peaks. The distance between the pole positions of the second and third highest quasiparticle peaks are nothing but the exchange splitting, which is easily calculated as $\Delta_x = \omega_0(1 - \lambda_2)$.

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