Quantum vortex dynamics from the microscopic Hamiltonian

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Starting with a microscopic Hamiltonian, we derive the Schrödinger equation of a superconductor with a vortex. The analysis describes the many-body state of a superconductor as a delocalized superposition of Bogoliubov-de Gennes mean-field vortex states. Taking a suitable one-band extended Hubbard model as the microscopic Hamiltonian of electrons in high-$T_c$ compounds, solutions to the vortex Schrödinger equation are computed. We compute the vortex mass. Tuning the Hamiltonian parameters, we obtain solutions for the case of an $s$-wave order parameter and for the $d$-wave case and consider consequences of order parameter symmetry for vortex directional motion.

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I. INTRODUCTION

For decades, researchers have studied the motion of vortices in type-II superconductors.\(^1\) This motion determines fundamental characteristics of superconductors, including critical current and mixed-state resistivity,\(^2\) which often dictate their technological usefulness. Because of the complicated nature of a vortex in a superconductor, however, many aspects of the theoretical understanding of vortex motion have remained incomplete. In particular, while magnetization measurements provide evidence that vortices in bulk superconductors can move via quantum tunneling, the theory of this quantum tunneling has been largely phenomenological in character. The strategy in the literature\(^3\)–\(^10\) has generally been to develop a classical equation of motion of the vortex center-of-mass as though a vortex were a point particle. Then, the equation of motion is expressed using a classical effective action. Finally, quantum tunneling rates are computed using the effective action. This “point-particle” approach has the virtue that it is tractable enough to yield analytical expressions for tunneling exponents and to permit the incorporation of complications such as dissipation. However, the correct form of the classical equation of motion has been a contentious question, and it is difficult to provide a firm justification for the subsequent quantization of the equation. Moreover, the result depends upon phenomenological parameters in the original equation of motion that are generally taken from experiment (however, see Ref. 11 and references therein).

In this paper, we approach the problem of vortex quantum motion from a microscopic quantum mechanical perspective. Our calculations are based on the Nambu-Gorkov equations of superconductivity; we do not require phenomenological vortex parameters and do not assume that the vortex can be treated as a point particle. Because of its microscopic foundation, the theory could potentially provide a foundation for quantitative, first principles analysis of vortex motion in real materials. It can also be utilized to address qualitative phenomena that are beyond the reach of effective vortex dynamics models. As a first such application, we consider vortices in high-$T_c$ superconductors. We compute the vortex mass and consider consequences of the $d$-wave nature of the order parameter\(^12,13\) that are difficult at best to analyze in other approaches.

We focus in this paper upon nondissipative motion, a topic that has elicited sustained theoretical concern even without the additional complication of dissipation.\(^14\)–\(^19\) Dissipation would be incorporated in the spirit of Ref. 20.

Our formulation works with the many-body state of a superconductor that has a large number $N$ of electrons. For simplicity, we assume that the electrons are confined to two dimensions, which is appropriate for a thin film or possibly a layered superconductor. To be concrete, in this paper we adopt the electronic Hamiltonian

$$H = \sum_{\langle ij \rangle \sigma} t_{ij} c_{i \sigma}^\dagger c_{j \sigma} - \mu \sum_\sigma n_{r, \sigma} + U \sum_i n_{r, \sigma}^i n_{r, -\sigma}^i$$

$$+ \frac{V}{2} \sum_{\langle ij \rangle, \sigma, \sigma'} n_{r, \sigma}^i n_{r, \sigma'}^j$$

that describes the motion of electrons in a square lattice of sites $i$ within a Cu-O plane of a high-$T_c$ superconductor.\(^21\) Here, $c_{r, \sigma}^\dagger$ creates an electron at position $r_i$ of spin $\sigma$; the number operator $n_{r, \sigma} = c_{r, \sigma}^\dagger c_{r, \sigma}$.

The brackets $\langle ij \rangle$ denote a sum over nearest neighbor sites. The nearest neighbor tunneling matrix elements are given by $t_{ij} = -t \exp \left[ i \left( \mathbf{r}_i - \mathbf{r}_j \right) \cdot \mathbf{A} / \hbar c \right]$, using the Peierls substitution to include the vector potential $A = -By$ of an applied magnetic field in the $z$ direction. This choice (1) will allow an interesting application of our formalism to the case of a $d$-wave superconductor. However, it will be evident in what follows that the formalism can accommodate a general class of Hamiltonians.

We denote the $N$ electron vortex state of the superconductor by $|v_N(0)\rangle$ where the 0 symbol indicates that the vortex is at the origin. To study the motion of the vortex, we consider the dynamics of the Hamiltonian in a basis of vortex states $|v_N(\mathbf{p})\rangle$, constructed by translating $|v_N(0)\rangle$ to all possible positions $\mathbf{p}$ in the lattice. The translations are achieved using a translation operator $T(\mathbf{p}) |v_N(\mathbf{p})\rangle = T(\mathbf{p}) |v_N(0)\rangle$.

In this basis, a time-dependent vortex state then takes the form $|\Psi(t)\rangle = \sum_{\mathbf{p}} |\Psi(\mathbf{p}, t)\rangle |v_N(\mathbf{p})\rangle$. While a vortex in Bogoliubov-de Gennes theory is an object localized at a single point, we now study its quantum dynamics by forming an
entirely delocalized vortex state. This is analogous to studying electron dynamics in a solid by forming a traveling Bloch wave of superposed Wannier states. To study vortex dynamics, we would like to evolve our state using the time-dependent Schrödinger equation

\[
H|\psi(t)\rangle = i\hbar \frac{d}{dt}|\psi(t)\rangle.
\]

To understand the evolution, in the usual way we can first compute the energy eigenstates \( |\phi\rangle = \sum_{\rho'} \psi_{\rho'}(\rho') \langle v_N(\rho') \rangle \) of the time-independent Schrödinger equation \((H-E)|\psi\rangle = 0\). In our basis, this equation is

\[
\sum_{\rho'} \langle v_N(\rho')|H-E|v_N(\rho')\rangle \psi(\rho') = 0.
\]

It is important to emphasize that we are not making a phenomenological point-particle assumption about the vortex coordinate \( \rho \) when we deal with states of the form \( |v_N(\rho)\rangle \). As is shown in Ref. 22, the vortex states satisfy variational minimization conditions; they are just low energy states of a superconductor in a magnetic field. Thus, our basis simply comprises the low-energy Hilbert space of the microscopic Hamiltonian. Physically, this basis is a natural choice for describing a superconductor with a moving vortex.

By carefully constructing the basis and analyzing its properties, we are able to solve the many-body Schrödinger equation (3). The construction of the basis is detailed in Sec. II. In Sec. III, we then derive formulas that enable us to evaluate the Hamiltonian matrix elements \( \langle v_N(\rho)|H|v_N(\rho')\rangle \) and the overlap \( \langle v_N(\rho)|v_N(\rho')\rangle \), keeping in mind that the states in our basis are not orthogonal. These matrix elements seem to require \( 2N \) dimensional many-body integrals, which can become intractable for even relatively small \( N \). In this paper, we provide tractable and somewhat intuitive forms for them by describing \( |v_N(\rho)\rangle \) using the mean-field, Nambu-Gorkov equations of superconductivity.\(^{26}\) Of course, a solution to (3) is then a delocalized superposition \( |\psi\rangle = \sum_{\rho'} \psi_{\rho'}(\rho') \langle v_N(\rho') \rangle \) of mean-field states, so that our approach cannot be derived within mean-field theory.\(^{26}\) In Sec. IV the matrix elements are evaluated numerically and the resulting Schrödinger equation (3) is studied. We compute the vortex mass and consider the effects of \( d \)-wave order parameter symmetry on vortex tunneling. The stability of the computation is also verified. Section V consists of concluding remarks.

II. BASIS OF VORTEX STATES

A. Bogoliubov-de Gennes theory

The Bogoliubov-de Gennes equations provide a good description of the state \( |v(0)\rangle \) of a superconductor that has a vortex at the origin and is in contact with a particle bath. This state can be well characterized using mean-field theory and the \( N \) electron state \( |v_N(0)\rangle \) can be obtained from it by projection \( |v_N(0)\rangle = P_N|v(0)\rangle \). Minimization of the expectation value of the Hamiltonian\(^{22}\) leads to the Bogoliubov-de Gennes equations

\[
\sum_j \left( \frac{(-i_j - \mu \delta_{ij})}{\Delta_{ij}^+} \right) \Delta_{ij} \left( \frac{(t_j + \mu \delta_{ij})}{\Delta_{ij}^+} \right) \langle u_{j n} | v_{j n} \rangle = E_n \langle u_{i n} | v_{i n} \rangle,
\]

where \( \mu \) is the chemical potential and where \( \Delta_{ij}^+ \) is the pair potential. We have omitted a Hartree-Fock potential along the diagonal since it should not play an important role in distinguishing the superconducting state from the normal state. We solve these equations numerically on a real-space lattice of size \( L_x \times L_y \) and lattice constant \( a \) following Wang and MacDonald.\(^{21}\) (See also Refs. 23–25 for an elegant alternate approach to solving the Bogoliubov-de Gennes problem in the vortex state.) This entails diagonalizing an \( N_o \times N_o \) matrix where \( N_o = 2L_x \times L_y / a^2 \) and the factor of 2 reflects the two components \( m \) and \( \bar{m} \) in (4). Physically, \( N_o \) is the number of single-particle states in the system including a factor of 2 for spin. For the Hamiltonian (1), the pair potential self-consistency equation is

\[
\Delta_{ij} = \sum_n U \delta_{r_i r_j} u_{i n} v_{j n} + \frac{V}{2} \delta_{r_i r_j} (u_{i n} v_{j n} + u_{j n} v_{i n}),
\]

where

\[
\delta_{r_i r_j} = \delta_{r_i r_j}^+ + \delta_{r_i r_j}^- + \delta_{r_i r_j}^+ + \delta_{r_i r_j}^- + \delta_{r_i r_j}^+ + \delta_{r_i r_j}^-,
\]

ensures that \( r_i \) and \( r_j \) are nearest neighbors in the square lattice, taking into account (magnetic) periodic boundary conditions with magnetic phase factors. (The form of the magnetic phase factors follows from the discussion below of the magnetic translation operator.) Given the solution to (4), quasiparticle destruction operators \( \gamma_{n,\sigma} \) are defined by the equations \( c_{r_i \sigma}^\dagger = \sum_n \gamma_{n,\sigma}^\dagger v_{i n} - \gamma_{n,\sigma} v_{i n}^\dagger \) and \( c_{r_i \sigma}^\dagger = \sum_n \gamma_{n,\sigma}^\dagger v_{i n} + \gamma_{n,\sigma} v_{i n}^\dagger \) following the conventions in Ref. 21. Then, the vortex state satisfies \( \gamma_{n}|v(0)\rangle = 0 \).

B. Nambu-Gorkov Green’s functions

Once we have the Bogoliubov-de Gennes mean-field solution that characterizes \( |v(0)\rangle \), the result can be conveniently expressed using Green’s functions. We define \( G_{s,s'}(r_i, r_{i'}, t) = \langle v(0)|T(d_{s,s'}(t), d_{s,s'}^\dagger(t')=0)|v(0)\rangle \) using a particle-hole transformation from the usual electron destruction operators to \( d_{s,s'} = e^{-i E_s d_{s,s'}} \) and \( d_{s,s'}^\dagger = e^{i E_s d_{s,s'}} \). For times \( t > 0 \), we find that

\[
\begin{pmatrix}
G_{1,1}(r_i, r_{i'}, t) & G_{1,-1}(r_i, r_{i'}, t) \\
G_{-1,1}(r_i, r_{i'}, t) & G_{-1,-1}(r_i, r_{i'}, t)
\end{pmatrix} = \sum_n \left( \frac{u_{i n}^*}{v_{i n}} \right) (u_{i n} v_{i n}^\dagger) e^{-i E_n d_{i,i'}}.
\]

Since the spatial coordinate ranges over \( N_o / 2 = L_x \times L_y / a^2 \) points and the spin coordinate ranges over two possibilities, at each instant of time \( G_{s,s'}(r_i, r_{i'}, t) \) is an \( N_o \times N_o \) matrix indexed by row \( (i,s) \) and column \( (j,s') \).

C. Magnetic translation operator

The vortex state \( |v_N(\rho)\rangle \) is obtained by translating \( |v_N(0)\rangle \), which contains a vortex at the origin. Because an external
vector potential $A(r) = -By\hat{z}$ breaks the translational symmetry in the tunneling elements $t_{ij}$ of (1), it is necessary to use magnetic translation operators. For single-particle wave functions, magnetic translation operators $\tau(p)$ are defined by $\tau(p)\psi(r) = e^{i(\pi B/2)\alpha r/\hbar}|\phi(r-p)\rangle$ where $\Phi_p = \hbar c/2|\epsilon|$ is the superconducting flux quantum. These operators are chosen so that they commute with the Hamiltonian. It is therefore possible for an eigenstate of the Hamiltonian to be a simultaneous eigenstate of $\tau(L_x,\hat{x})$ or of $\tau(L_y,\hat{y})$. Moreover, an eigenstate of the Hamiltonian can be a simultaneous eigenstate of both $\tau(L_x,\hat{x})$ and $\tau(L_y,\hat{y})$ as long as $[\tau(L_x,\hat{x}),\tau(L_y,\hat{y})] = 0$. This commutator vanishes provided that $e^{i(\pi B/2)\alpha r/L_x}$, $e^{i(\pi B/2)\alpha r/L_y} = 1$, which means that the flux through the system satisfies $BL_x L_y = 2n\Phi_0$ for $n$ an integer. The eigenvalue equations become Born-von Karman-type boundary conditions $\tau(L_x,\hat{x})\psi(r) = \psi(r)$ and $\tau(L_y,\hat{y})\psi(r) = \psi(r)$ if we require unit eigenvalues.

Using the translation operator $\tau(p)$, we would like to be able to operate upon an eigenstate $\psi(r)$ of the Hamiltonian that satisfies the boundary conditions and obtain another eigenstate of the Hamiltonian that satisfies the boundary conditions. This requires that $[\tau(p),\tau(L_x,\hat{x})] = [\tau(p),\tau(L_y,\hat{y})] = 0$. The commutators vanish provided that $e^{i(\pi B/2)\alpha r/L_x,\alpha p} = 1$. In order to permit the smallest translations $\rho = \pm \alpha\hat{x}$ and $\rho = \pm \alpha\hat{y}$, it is necessary that the system be large enough so that $L_x$ and $L_y$ satisfy $BL_x L_y = 2n\Phi_0$ and $BL_x, L_y = 2n\Phi_0$ for integral $n_x$ and $n_y$. In this case, our Born-von Karman boundary conditions $\tau(L_x,\hat{x})\psi(r) = \psi(r)$ and $\tau(L_y,\hat{y})\psi(r) = \psi(r)$ become the usual periodic boundary conditions. If it is not feasible to calculate using such large systems, as long as $BL_x L_y = 2n\Phi_0$ for $n$ one can get results by approximating that the system characteristics are constant throughout the magnetic Brillouin zone.

Having derived these conditions on the system size, we now need to generalize $\tau(p)$ to an operator $T(p)$ that takes a many-body state $\psi(r_1,\ldots,r_N)$ to $\prod e^{i(\pi B/2)\alpha(r_i-r_j/2)}\psi(r_1-r_\rho,\ldots,r_N-r_\rho)$. In creation operator notation, we have

$$T(p) = \prod_{r,s} \langle C_{r,s} C_{r,s}^\dagger + C_{r,s}^\dagger C_{r,s} \rangle \times \prod_{r,s} \langle C_{r,p} C_{r,p}^\dagger + e^{i(\pi B/2)p_x/\hbar}(x_{r,p}/2) C_{r,p}^\dagger \rangle$$

for arbitrary $n$. A form that works for arbitrary $n$ is

$$T(p) = \prod_{R,S} \langle C_{R,S} C_{R,S}^\dagger + C_{R,S}^\dagger C_{R,S} \rangle \times \prod_{r,s} \langle C_{r,p} C_{r,p}^\dagger + e^{i(\pi B/2)p_x/\hbar}(x_{r,p}/2) C_{r,p}^\dagger \rangle$$

In this expression we have introduced fermionic operators of the form $C_{r,s}$ that create electrons in a fictitious auxiliary space. Inspecting the form of $T(p)$ from right to left, we see that it considers each location $r - \rho, s$ in the lattice. If an electron is present, that electron is placed in the auxiliary space at $r, s$, and its state is multiplied by the magnetic phase factor $e^{i(\pi B/2)p_x/\hbar}(x_{r,p}/2)$. If no electron is present, nothing is done. Once every location has been considered, the electrons are simply carried from the auxiliary space back to the original space, emptying the auxiliary space once again. (The auxiliary space is necessary because one cannot directly shift an electron from $r - \rho$ to $r$ without first placing any electrons already in $r$ into some kind of holding box.)

Making a particle-hole transformation on the electron operators and also on the “holding-space” operators $(D_{R,1} = C_{R,1}$ and $D_{R,-1} = C_{R,-1})$, we find

$$T(p) = (\pm 1)^{\rho_x/2} \prod_{R,S} \langle D_{R,S} D_{R,S}^\dagger + D_{R,S}^\dagger D_{R,S}\rangle \times \prod_{r,s} \langle d_{r,s} d_{r,s}^\dagger + e^{i(\pi B/2)p_x}(x_{r,s}/2) D_{r,s}^\dagger d_{r,s}\rangle \times \prod_{r} D_{r,-1},$$

\[ \text{(7)} \]

as is derived in Appendix A. To obtain the leading phase factor, we have written $e^{i(\pi B/2)p_x}(x_{r,s}/2) = (\pm 1)^{\rho_x/2}$ with the sign depending upon whether $e^{i(\pi B/2)p_x}(x_{r,s}/2) = \pm 1$. In any case, the factor can be absorbed into the definition of the vortex state if desired, as $|\psi(p)\rangle = (\pm 1)^{\rho_x/2} T(p) |\psi(0)\rangle$, and can therefore be omitted from the translation operator.

Knowing $T(p)$ and $|\psi(0)\rangle$, it is possible to construct the basis of vortex states $\{|\psi_n(0)\rangle\}$. One needs only to have a way to apply a number projection$^{29}$ to obtain $|\psi_n(0)\rangle = P_N|\psi(0)\rangle$. It is particularly convenient to incorporate the projection operator $P_N$ into $T(p)$ as follows:

$$T(p) = \frac{N}{2\pi} \int \frac{dN}{2\pi} e^{-i\theta_N} \prod_{R,S} \langle C_{R,S} C_{R,S} + C_{R,S}^\dagger C_{R,S}\rangle \times \prod_{r,s} \langle C_{r,p} C_{r,p} + e^{i(\pi B/2)p_x}(x_{r,p}/2) C_{r,p}^\dagger \rangle$$

since the integral selects out terms with exactly $N$ destruction operators $C_{r,p}$. The particle-hole transformation is executed for $T(p)P_N$ just as for $T(p)$. An additional phase factor $e^{i(\pi N/2)}$ arises

$$T(p)P_N = (\pm 1)^{\rho_x/2} \prod_{R,S} \langle D_{R,S} D_{R,S}^\dagger + D_{R,S}^\dagger D_{R,S}\rangle \times \prod_{r,s} \langle d_{r,s} d_{r,s}^\dagger + e^{i(\pi B/2)p_x}(x_{r,s}/2) D_{r,s}^\dagger d_{r,s}\rangle \prod_{r} D_{r,-1},$$

\[ \text{(8)} \]

where we have used the fact that $L_x L_y = 2N_x/2$.

III. MATRIX ELEMENTS

A. Determinant formulas

Having derived the forms of $T(p)$ and $T(p)P_N$, one can evaluate the overlap matrix element $\langle \psi_n(p) | \psi_m(p) \rangle = \langle \psi_n(p) | P_N T(p) T(p)^\dagger P_N | \psi_m(p) \rangle$ and the Hamiltonian matrix element $\langle \psi_n(p) | H | \psi_m(p) \rangle = \langle \psi_n(p) | P_N T(p) H T(p)^\dagger P_N | \psi_m(p) \rangle$ that appear in Eq. (3). Since $P_N$ is a projection operator satisfying $P_N^2 = P_N$, we can simplify $P_N T(p) T(p)^\dagger P_N = T(p) T(p)^\dagger P_N = T(p)^2 P_N$. This reduces the overlap matrix element to
\[ \langle v_N(\rho) | v_N(\rho') \rangle = \langle v(0) | T'(\rho) T(\rho') P_N | v(0) \rangle. \]
Similarly, the Hamiltonian matrix element is
\[ \langle v_N(\rho) | H | v_N(\rho') \rangle = \langle v(0) | T(\rho^H) T'(\rho') P_N | v(0) \rangle. \]

The overlap can be evaluated by invoking the forms (7) and (8) and performing a cumbersome Wick’s theorem calculation. The argument is presented in detail in Appendix B; here we present the result
\[
\langle v_N(\rho) | v_N(\rho') \rangle = \int \frac{d\chi}{2\pi} e^{i\left(N(N/2-N)\chi \right)} \det M(\chi),
\] (9)
where we have defined an \( N_o \times N_o \) matrix \( M \) indexed by row \((r,s)\) and column \((r',s')\) with matrix elements
\[ M(\chi)_{(r,s);(r',s')} = -G_{r,s}(r-\rho',r'-\rho,t=0^+) + G_{r',s}(r-\rho',r'-\rho,t=0^-) \times e^{i\chi \left[ \epsilon_n^{(s)}(s'-(s'-p)/2) - \epsilon_n^{(s)}(s'-p)/2) \right]}. \]
(10)

An intuitive interpretation of the results (9) and (10) can be obtained by analogy to a simpler case. Imagine that the magnetic field were absent and that \( |v_N(0)\rangle \) were, instead of a superconducting vortex state, a Hartree-Fock state of \( N \) spinless fermions in a Hilbert space of total dimension \( N_o^N \). In that case, \( |v_N(0)\rangle \) would be a Slater determinant of \( N \) orbitals, \( \zeta_n(r) (n=1,...,N) \) drawn from a complete, orthonormal basis of \( N \) orbitals, \( \zeta_n(r) (n=1,...,N_o) \). It would follow from the definition of the Slater determinant that \( \langle v_N(\rho) | v_N(\rho') \rangle \)
\[ = \det Z, \]
for \( Z \) an \( N \times N \) matrix of overlap integrals \( Z_{m,n} = \int dr \zeta_m^{(s)}(r-\rho) \zeta_n^{(s)}(r-\rho) \). We can show that \( \det Z = \det M \) where \( M \) is an \( N_o \times N_o \) matrix with elements
\[ M_{r,r'} = -G(r-\rho',r'+\rho',t=0^+) + G(r-\rho',r'+\rho,t=0^-) \]
(11)
containing the retarded and advanced Green’s functions
\[ G(r,r'+\rho',t=0^+) = \sum_{s=1}^{N_o} \xi_n^{(s)}(r) \xi_n^{(s)}(r') \]
and
\[ G(r,r'+\rho,t=0^-) = \sum_{s=1}^{N_o} \zeta_n^{(s)}(r) \zeta_n^{(s)}(r'). \]

To demonstrate that \( \det Z = \det M \), we simply make a unitary transformation \( U \) from the real space basis to the \( \zeta \) basis by taking \( U_{r,s} = \tilde{\zeta}_n(r-\rho) \). One finds that
\[ U.M.U^\dagger = \tilde{Z} \]
where
\[ \tilde{Z} = \int dr \sum_{m,n} \zeta_m^{(s)}(r-\rho) \zeta_n^{(s)}(r+\rho'), \]

using the sum form above of the Green’s functions. Writing out \( Z \) and \( \tilde{Z} \) one readily sees that \( \det Z = \det \tilde{Z} \) so that
\[ \det Z = \det \tilde{Z} = \det U.M.U^\dagger = \det M. \]

We conclude that
\[ \langle v_N(\rho) | v_N(\rho') \rangle = \det M \]
(12)
which together with (11) is clearly reminiscent of (9) and (10), although the latter are more complicated because they also incorporate a magnetic field and integrate to effect a number projection \( P_N \). The formula (11) has an intuitive appeal, since the \( G(r-\rho',r'+\rho,t=0^+) \) part leaves the \( N \) occupied orbitals in \( |v_N(\rho')\rangle \) from \( \rho' \) to \( \rho \) while the
\[ G(r-\rho',r'-\rho',t=0^-) \] part leaves the \( N_o-N \) unoccupied orbitals untranslated.

Terms required for computing the Hamiltonian matrix element \( \langle v_N(\rho) | H | v_N(\rho') \rangle \)
\[ = \langle v(0) | T(\rho^H) T'(\rho') P_N | v(0) \rangle \]
are computed in Appendix C. Considering the form of the Hamiltonian (1), the following formulas are sufficient:
\[
\langle v_N(\rho) | d_{\tau_1,\tau'_1}^l d_{\tau_2,\tau'_2}^l | v_N(\rho') \rangle
= \int \frac{d\chi}{2\pi} e^{i\left(N(N/2-N)\chi \right)} \det M(d_{\tau_1,\tau'_1}^l d_{\tau_2,\tau'_2}^l),
\]
(13)
where \((\tau_1,\tau'_1) \neq (\tau_2,\tau'_2)\) and where
\[ M(d_{\tau_1,\tau'_1}^l d_{\tau_2,\tau'_2}^l) = M(\chi)_{(\tau_2,\tau'_2),(\tau_1,\tau'_1)} (1 - \delta_{\tau_1,\tau_2} \delta_{\tau'_1,\tau'_2}) + G_{\tau_1,\tau_2}(r-\rho',r-\rho,t=0) \times e^{i\chi \left[ \epsilon_n^{(s)}(s'-(s'-p)/2) - \epsilon_n^{(s)}(s'-p)/2) \right]} \times (\delta_{\tau_1,\tau_1}(s')) \delta_{\tau_2,\tau_2}(s_2), \]
(14)
Equations (1), (3), (9), (10), (13), and (14) provide the ingredients for a microscopic calculation of quantum vortex dynamics. We stress that, although the formulas are complicated in appearance, intuitive insight into their form has been provided from the Hartree-Fock case. Most importantly, they are attractive and manageable from a computational standpoint. Each of these equations expresses a many-body matrix element as the integral over \( \chi \) of the determinant of an \( N_o \times N_o \) matrix that depends upon \( \chi \). They replace unmanageable \( 2N \) dimensional many-body integrals for \( \langle v_N(\rho) | v_N(\rho') \rangle \) and \( \langle v_N(\rho) | H | v_N(\rho') \rangle \) with determinants and a single dimensional integral. The result is a computationally tractable formalism evaluated below for \( N \) up to 310.
B. Translational behavior of matrix elements

The position dependence of the matrix elements can be simplified. We focus upon the overlap. As found in Sec. II C, the system obeys periodic boundary conditions on the $L_x \times L_y$ lattice. We can therefore shift the value of $r$ in matrix element (14) by $L_x \tilde{x}$ or by $L_y \tilde{y}$ without changing the value of the matrix element. Thus, in the matrix $M$ we can think of the $x$ component of $r$ as running not from $a, \ldots, \rho_x', -a, \rho_x', \ldots, L_x$ but instead as running from $(\rho_x' + a), \ldots, (L_x + \rho_x' - a), \rho_x', \ldots, L_x$. Similarly, the $y$ component can be made to run from $(\rho_x' + \rho_y')$, \ldots, $(L_y + \rho_x' - \rho_y')$, $\rho_y', \ldots, L_y$. We can do the same thing to the column index $r'$. Then, without changing the value of $\det M$, we can reorder the rows and columns so that the $x$ component of $r$ runs from $\rho_x', \ldots, L_x + \rho_x'$, the $y$ component of $r$ runs from $\rho_y', \ldots, L_y + \rho_y'$, and similarly for $r'$. Thus,

$$\det M(\chi_{(r';x')}) \equiv \det M(\chi_{(r'+p',y')})$$

where the matrix element

$$M(\chi_{(r';x')}) = e^{-i(\chi_{(r+p',y')})} \times \left[G_{x,x'}(\rho', \rho_x', t = 0') + G_{y,y'}(\rho', \rho_y', t = 0') \times e^{-i(\chi_{(\rho_y' + \rho_x')})}\right]$$

Defining $\chi = \chi + \pi B/\Phi_0$, $\rho_x'/2 - \rho_y' \rho_x'/2$ as a new variable of integration, we find that

$$\langle v_N(\rho') | v_N(\rho') \rangle = \int e^{i(N_v/2-N)\chi} \langle \chi-\pi B/\Phi_0 \rangle \rho_x'/2 - \rho_y' \rho_x'/2 \rangle \times G_{x,x'}(\rho', \rho_x', t = 0') + G_{y,y'}(\rho', \rho_y', t = 0') \times e^{-i(\chi_{(\rho_y' + \rho_x')})}\right] \frac{d\chi}{2\pi}$$

$$= e^{i(N_v/2-N)\pi B/\Phi_0} \rho_x'/2 - \rho_y' \rho_x'/2 \rangle \times \langle v_N(\rho' - \rho') | v_N(0) \rangle.$$}

Similarly, we can show that

$$\langle v_N(\rho') | H | v_N(\rho') \rangle = e^{i(N_v/2-N)\pi B/\Phi_0} \rho_x'/2 - \rho_y' \rho_x'/2 \rangle \times \langle v_N(\rho' - \rho') | H | v_N(0) \rangle.$$}

Thus, the matrix elements are translationally invariant except for the presence of a magnetic phase factor. The phase factor is simply that of system of charge $-N|e|$ moving in a magnetic field $B$, where $N$ is the number of electrons in the system. The phase proportional to $N_v/2$ is simply an artifact of the factors of $(\pm 1)^{\rho_x' \rho_x'/2} T(\rho)$ introduced into the definition in Sec. II C above $|v(\rho') = (\pm 1)^{\rho_x' \rho_x'/2} T(\rho) | v(0) \rangle$; this phase has no physical significance and can be removed if the factors are removed from the definition.] Our argument did not depend on the detailed form of the Green’s functions so the conclusion is quite reasonable and generic. And since only the product of the charge and the magnetic field enter the phase factor, we can alternatively understand the phase as

describing the force on vortices of charge $-|e|$ each moving in a magnetic field of size $n \Phi_0$, where $n$ is the density of electrons in the system. Whether effects of this type are best termed Lorentz forces or Magnus forces has been the subject of some debate.\textsuperscript{17} In any case, when one solves the Schrödinger equation (3) the quantum states of the vortex will roughly take the form of Landau levels.

Since the vortex states are not orthogonal, it can be convenient to transform to an orthogonal basis before solving (3). If we define the Hermitian overlap matrix $O_{\rho,\rho'} = \langle v_N(\rho') | v_N(\rho') \rangle$, the new basis

$$|b(\rho') = \sum_{\rho'} O_{\rho,\rho'} | v_N(\rho') \rangle$$

is orthonormal (assuming that the matrix $O^{-1/2}$ exists). In the new basis, the Hamiltonian matrix $H_{\rho,\rho'} = |v_N(\rho') | H | v_N(\rho') \rangle$, becomes $O^{-1/2} H O^{-1/2}$, and we solve (3) by simply diagonalizing this new Hamiltonian.

IV. LANDAU LEVEL DESCRIPTION OF VORTEX STATE

This formalism makes it possible to study subtle aspects of vortex dynamics, such as consequences of $d_{2s-2d}$-wave order parameter symmetry in a high-$T_c$ superconductor. We follow Ref. 21 and solve the Bogoliubov-de Gennes equations (4) self-consistently, where the parameters $t$, $\mu$, $U$, and $V$ in (1) are chosen appropriately for a cuprate with $d$-wave order parameter symmetry. We then use our solution to obtain Nambu-Gorkov Green’s functions (6).

Next, we evaluate the overlap matrix elements using (9) and (10). Figure 1 plots the magnitude of the calculated overlap $|\langle v_N(\rho = X \tilde{x} + Y \tilde{y}) | v_N(0) \rangle|$ as a function of displacement $X$ and $Y$ in units of the lattice constant $a$. Calculations are made on a $14 \times 28$ real-space lattice ($N_v = 2 \times 14 \times 28 = 784$), where the number $N = 0.8 (N_v/2) = 310$ of electrons in the superconductor is set near optimal doping.\textsuperscript{21} The results exhibit Gaussian fall off as a function of distance. As a result, one can justify neglecting all overlap and Hamiltonian matrix elements beyond nearest neighbor.

The stability of our overlaps is a concern considering the instability of normal state overlaps obtained in orthogonality catastrophe calculations.\textsuperscript{20,33} The nearest neighbor and next nearest neighbor overlaps appearing in Fig. 1 do not appear.
to depend sensitively upon the 14 × 28 lattice size used in the numerical calculation. To demonstrate this, Fig. 2 displays the nearest neighbor and next nearest neighbor overlaps for lattices of increasing size. Note that the magnitude of the overlap changes little even when the number of electrons grows by more than a factor of 3. This is not a proof of stability, but it is an encouraging indicator. Overlaps between more distant neighbors exhibit more instability as we increase the lattice size, although they fall off with distance as a Gaussian and therefore are usually much less physically important.

In order to complete the specification of the time-independent Schrödinger equation (3), it is necessary to compute the Hamiltonian matrix elements $\langle \psi_N(\mathbf{p}) | H | \psi_N(\mathbf{p}') \rangle$. Because of the sums over lattice positions in (1), the Hamiltonian matrix element calculations are substantially more demanding than the overlap calculations of Fig. 1. Since the results of Fig. 2 suggest that smaller lattices may yield reasonable results, we proceed using a 8 × 16 real-space lattice ($N_e = 256$), where the number $N = 0.8(N_e/2) = 102$ of electrons in the superconductor is set near optimal doping.

After evaluating the matrix elements (13), tunneling matrix elements in (3) between nearest neighbor lattice sites $\mathbf{p} = \mathbf{p'} \pm \pm \bar{x}$ or $\mathbf{p} = \mathbf{p'} \pm \pm \bar{y}$ are found to be of order $1 \times 10^{-1}$. (Note that the word “tunneling” is used here to refer to matrix elements between sites on a lattice; it is not intended to connote tunneling from one side of an applied potential barrier to the other side.) Since the effective mass of a particle on a lattice is inversely proportional to its tunneling matrix elements, and since $\tau = |t_i|$ is the magnitude of the tunneling matrix elements in (1), the vortex mass is $\sim 10$ times the electron mass. This agrees with predictions of order the electron mass density times the vortex core size discussed in articles such as Ref. 18. Calculations performed using an $s$-wave order parameter yield smaller ($\sim 20\%$ smaller) tunneling matrix elements than those obtained using an $d_{z^2}$-wave order parameter. The relative importance of diagonal tunneling by $\mathbf{p} = \mathbf{p'} \pm \pm \bar{x}$ to next nearest neighbors is enhanced ($\sim 20\%$ in the $s$-wave case compared to the $d_{z^2}$-wave case. It appears that the presence of order parameter nodes inhibits tunneling along the diagonal. Although there have been calculations of properties like the vortex mass in a $d_{z^2}$-wave system (e.g., Ref. 32), the directional preference of vortex quantum tunneling in this system has not been investigated before in the literature to our knowledge. In-depth numerical studies on larger lattices will be valuable in exploring this observation further.

For some calculations, it may be sufficient to study the semiclassical limit of our theory of vortex quantum dynamics. We have seen that the vortex Hamiltonian to first approximation has the form of a charged particle in a magnetic field. By applying WKB theory to, say, tunneling of this particle through a barrier, one can obtain a semiclassical description of the vortex motion. The analysis will then be comparable to the point-particle approximation of Refs. 3–10.

V. CONCLUDING REMARKS

This paper has presented a microscopic approach to quantum vortex dynamics based upon the Schrödinger equation (3) and the matrix element formulas (9) and (13). Applying this methodology to a reasonable Hamiltonian (1) for one plane of a cuprate, we have computed a vortex mass on the order of 10 electron masses. The $d$-wave symmetry of the order parameter appears to suppress tunneling along order parameter nodal lines. Although we have focused on (1), the formalism can be applied to tight-binding type Hamiltonians quite generally. For instance, the formulas (13) permit the inclusion of a potential $\Sigma_{r,s} V(r,s) c_{r,s}^\dagger c_r$ of the lattice, with or without impurities.

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APPENDIX A: PARTICLE-HOLE TRANSFORMATION

It is convenient to introduce a particle-hole transformation in the translation operator. The $S = s = -1$ factors in $T(\mathbf{p})$ are

$$\prod_{\mathbf{R}} (C_{\mathbf{R} - \mathbf{1}} c_{\mathbf{R} - \mathbf{1}}^\dagger + e^{i(\pi B/4)\tilde{R}p_z(s - p_z/2)} C_{\mathbf{R} - \mathbf{1}} c_{\mathbf{R} - \mathbf{1}}^\dagger)$$

$$\times \prod_{\mathbf{R}} (C_{\mathbf{R} - \mathbf{1}} c_{\mathbf{R} - \mathbf{1}}^\dagger - e^{i(\pi B/4)\tilde{R}p_z(s - p_z/2)} C_{\mathbf{R} - \mathbf{1}} c_{\mathbf{R} - \mathbf{1}}^\dagger)$$

$$\times \prod_{\mathbf{R}} (e^{i(\pi B/4)\tilde{R}p_y(s - p_y/2)} c_{\mathbf{R} - \mathbf{1}} c_{\mathbf{R} - \mathbf{1}}^\dagger)$$

$$\times \prod_{\mathbf{R}} (c_{\mathbf{R} - \mathbf{1}} c_{\mathbf{R} - \mathbf{1}}^\dagger - e^{-i(\pi B/4)\tilde{R}p_y(s - p_y/2)} c_{\mathbf{R} - \mathbf{1}}^\dagger c_{\mathbf{R} - \mathbf{1}})$$

$$\times \prod_{\mathbf{R}} e^{i(\pi B/4)\tilde{R}p_y(s - p_y/2)} c_{\mathbf{R} - \mathbf{1}}^\dagger c_{\mathbf{R} - \mathbf{1}}$$
\[= (e^{i(\pi B/2\psi_0)\rho_1,\rho_1}) C_{\rho_1} \cdot C_{\rho_1} \prod_{r} C_{\rho_{r-1}} \]
\[
\times \prod_{r} (C_{\rho_{r-1}} C_{\rho_{r-1}} + c_{\rho_{r-1}} C_{\rho_{r-1}}) 
\times \prod_{r} (c_{\rho_{r-1}} e_{\rho_{r-1}} + e^{-i(\pi B/2\psi_0)\rho_1,\rho_1} C_{\rho_{r-1}} c_{\rho_{r-1}} - 1) \prod_{r} C_{\rho_{r-1}}.
\]

The phase factor at the beginning arises since our boundary conditions imply and this last factor is unity \(\prod_{r} e^{i(\pi B/2\psi_0)\rho_1,\rho_1 \cdot 2} = 1\). A particle-hole transformation then leads to (7).

**APPENDIX B: OVERLAP MATRIX ELEMENTS**

We derive here the overlap matrix elements equations (9) and (10). Inserting (7) and (8), we note that

\[
\langle v_N|p\rangle = \langle v_0|T(p)|T(p')P_N|v_0\rangle.
\]

\[
= \int \frac{d\chi}{2\pi} e^{i(N/2-N)\chi} \langle v(0)| \left( \prod_{r} D_{\rho_{r-1}}^\dagger \right) \prod_{r,s} (d_{\rho_{r-1},\rho_{s-1}} d_{\rho_{s-1},\rho_{r-1}} + e^{-i(\pi B/2\psi_0)\rho_1,\rho_1} d_{\rho_{r-1},\rho_{s-1}} D_{\rho_{s-1}}) \prod_{R,S} \left( D_{R,S} d_{R,S} + d_{R,S}^\dagger D_{R,S}^\dagger \right) \right| v(0) \rangle
\]

\[
\times \prod_{r} (D_{\rho_{r-1}}) \left( \prod_{r'} D_{\rho_{r-1}}^\dagger \right) \prod_{r',s'} \left( D_{R',S'} d_{R',S'}^\dagger + d_{R',S'} D_{R',S'}^\dagger \right) \prod_{r'} \left( D_{r'} D_{r'}^\dagger \right) |v(0)\rangle.
\]

To evaluate this, we start by noticing that the middle factors \((\prod_{R} D_{R}) (\prod_{R'} D_{R'}^\dagger)\) give unity when acting to the left or the right. With these operators eliminated, we consider the new middle factors

\[
\prod_{R,S} \left( D_{R,S} d_{R,S} + d_{R,S}^\dagger D_{R,S}^\dagger \right) \prod_{R',S'} \left( D_{R',S'} d_{R',S'}^\dagger + d_{R',S'} D_{R',S'}^\dagger \right) \to 1
\]

since \(d_{R,S}\) yields zero when it acts to the right, \(d_{R,S}^\dagger\) yields zero when it acts to the left, and \(d_{R,S}^\dagger d_{R,S}\) yields unity. This leaves

\[
\langle v_N|p\rangle = \int \frac{d\chi}{2\pi} e^{i(N/2-N)\chi} \langle v(0)| \left( \prod_{r} D_{\rho_{r-1}} \right) \prod_{r,s} (d_{\rho_{r-1},\rho_{s-1}} d_{\rho_{s-1},\rho_{r-1}} + e^{-i(\pi B/2\psi_0)\rho_1,\rho_1} d_{\rho_{r-1},\rho_{s-1}} D_{\rho_{s-1}}) \right| v(0) \rangle
\]

\[
\times \prod_{r} \left( D_{\rho_{r-1}} \right) \left( \prod_{r'} D_{\rho_{r-1}}^\dagger \right) \prod_{r',s'} \left( D_{r',s'} d_{r',s'}^\dagger + e^{-i(\pi B/2\psi_0)\rho_1,\rho_1} d_{r',s'} D_{r',s'}^\dagger \right) \prod_{r'} \left( D_{r'} D_{r'}^\dagger \right) |v(0)\rangle.
\]

We can expand the first product over \(r,s\) as a sum

\[
= \int \frac{d\chi}{2\pi} e^{i(N/2-N)\chi} \langle v(0)| \left( \prod_{r} D_{\rho_{r-1}} \right)
\]

\[
\times \sum_{n=0}^{N_r} \sum_{\{r_1, s_1\} \ldots \{r_n, s_n\}} \left( e^{-i(\pi B/2\psi_0)\rho_1,\rho_1} d_{r_1, s_1} \ldots e^{-i(\pi B/2\psi_0)\rho_1,\rho_1} d_{r_n, s_n} D_{r_n, s_n} \right)
\]

\[
\times \prod_{r, s'} \left( d_{r, s'} d_{r, s'}^\dagger + e^{-i(\pi B/2\psi_0)\rho_1,\rho_1} d_{r, s'} D_{r', s'}^\dagger d_{r', s'} \right) \prod_{r'} \left( D_{r'} D_{r'}^\dagger \right) |v(0)\rangle.
\]
where the locations \((\mathbf{r}_1, s_1), \ldots, (\mathbf{r}_n, s_n)\) in the sum are all distinct and where only one of the \(n!\) permutations of these locations contributes to the sum.

The operator \(D_{r,s_i}\) must be paired with \(D_{r,s_j}^\dagger\) or it will annihilate the state \((\Pi_r D_{r,-s_i})|v(0)\rangle\). The result is

\[
\langle v(0)|\left(\prod_{r} D_{r,-p_{r}}^\dagger\right)\langle v(0)|v(0)\rangle = \int \frac{d\chi}{2\pi} e^{i\chi(N/2-N)} \sum_{\mathbf{r},s} \sum_{n=0}^{N_{\mathbf{r},s}} \langle v(0)|\left(e^{-i\delta\chi(\pi B_0)\delta_y(s_1-p_{r}')}d_{r,-p_{r}}^\dagger \cdots e^{-i\delta\chi(\pi B_0)\delta_y(s_n-p_{r}')}d_{r,-p_{r}}^\dagger\right)|v(0)\rangle.
\]

Invoking Wick’s theorem, this leaves us with a sum over permutations \(P\),

\[
\langle v(0)|\left(\prod_{r} D_{r,-p_{r}}^\dagger\right)\langle v(0)|v(0)\rangle = \int \frac{d\chi}{2\pi} e^{i\chi(N/2-N)} \sum_{\mathbf{r},s} \sum_{n=0}^{N_{\mathbf{r},s}} \langle v(0)|\left(e^{-i\delta\chi(\pi B_0)\delta_y(s_1-p_{r}')}d_{r,-p_{r}}^\dagger \cdots e^{-i\delta\chi(\pi B_0)\delta_y(s_n-p_{r}')}\right)|v(0)\rangle
\]

The symbol \((-1)^P\) is +1 for even permutations and −1 for odd permutations. In the second to last equality, the sum over permutations is written as a determinant. The result (9) follows from definition (10) of \(\mathcal{M}\).

**APPENDIX C: HAMILTONIAN MATRIX ELEMENTS**

The analysis of \(\langle v_N(\mathbf{p})|v_N(\mathbf{p}')\rangle\) can be extended to yield Hamiltonian matrix element formulas (13) and (14),

\[
\langle v_N(\mathbf{p})|H|v_N(\mathbf{p}')\rangle = \sum_{ij} -t_{ij} \langle v_N(\mathbf{p})|c_{i\mathbf{r}',\sigma}\mathbf{c}_{j\mathbf{r}}^\dagger|v_N(\mathbf{p}')\rangle - \mu \sum_i \langle v_N(\mathbf{p})|n_{i\mathbf{r},\sigma}|v_N(\mathbf{p}')\rangle + U \sum_i \langle v_N(\mathbf{p})|n_{i\mathbf{r},\sigma}|v_N(\mathbf{p}')\rangle
\]

\[
+ \frac{V}{2} \sum_{ij,\sigma'\sigma} \langle v_N(\mathbf{p})|n_{i\mathbf{r},\sigma}n_{j\mathbf{r}',\sigma'}|v_N(\mathbf{p}')\rangle
\]

\[
= \sum_{ij} -t_{ij} \langle v_N(\mathbf{p})|d_{i\mathbf{r},\sigma}^\dagger d_{i\mathbf{r},\sigma}|v_N(\mathbf{p}')\rangle - \mu \sum_i \langle v_N(\mathbf{p})|d_{i\mathbf{r},\sigma}^\dagger d_{i\mathbf{r},\sigma}|v_N(\mathbf{p}')\rangle
\]

\[
+ U \sum_i \langle v_N(\mathbf{p})|(1 - d_{i\mathbf{r},\sigma}^\dagger d_{i\mathbf{r},\sigma})|v_N(\mathbf{p}')\rangle + \frac{V}{2} \sum_{ij} \langle v_N(\mathbf{p})|(1 - d_{i\mathbf{r},\sigma}^\dagger d_{i\mathbf{r},\sigma})|v_N(\mathbf{p}')\rangle
\]

The first needed matrix element is

\[
\langle v_N(\mathbf{p})|d_{i\mathbf{r},\sigma}^\dagger d_{i\mathbf{r},\sigma}|v_N(\mathbf{p}')\rangle = \int \frac{d\chi}{2\pi} e^{i\chi(N/2-N)} \langle v(0)|\left(\prod_{r} D_{r,-p_{r}}^\dagger\right)\langle v(0)|v(0)\rangle
\]

\[
\times \prod_{r,s} (D_{r,s}^\dagger D_{r,s} + D_{r,s}^\dagger D_{r,s}^\dagger) \left(\prod_{r} D_{r,-p_{r}}^\dagger\right) \langle v(0)|v(0)\rangle
\]

\[
\times \prod_{r,s} (D_{r,s}^\dagger D_{r,s} + D_{r,s}^\dagger D_{r,s}^\dagger) \left(\prod_{r'} D_{r',-p_{r'}}^\dagger\right) \langle v(0)|v(0)\rangle
\]

\[
\times \prod_{r,s} (D_{r,s}^\dagger D_{r,s} + D_{r,s}^\dagger D_{r,s}^\dagger) \left(\prod_{r'} D_{r',-p_{r'}}^\dagger\right) \langle v(0)|v(0)\rangle
\]

\[
\times \prod_{r,s} (D_{r,s}^\dagger D_{r,s} + D_{r,s}^\dagger D_{r,s}^\dagger) \left(\prod_{r'} D_{r',-p_{r'}}^\dagger\right) \langle v(0)|v(0)\rangle
\]

\[
\times \prod_{r,s} (D_{r,s}^\dagger D_{r,s} + D_{r,s}^\dagger D_{r,s}^\dagger) \left(\prod_{r'} D_{r',-p_{r'}}^\dagger\right) \langle v(0)|v(0)\rangle
\]

\[
\times \prod_{r,s} (D_{r,s}^\dagger D_{r,s} + D_{r,s}^\dagger D_{r,s}^\dagger) \left(\prod_{r'} D_{r',-p_{r'}}^\dagger\right) \langle v(0)|v(0)\rangle
\]

\[
\times \prod_{r,s} (D_{r,s}^\dagger D_{r,s} + D_{r,s}^\dagger D_{r,s}^\dagger) \left(\prod_{r'} D_{r',-p_{r'}}^\dagger\right) \langle v(0)|v(0)\rangle
\]
Almost identical reasoning yields the two-body matrix element,

\[ \langle \Psi_N | \hat{D}_{r,s} | \Psi_N \rangle = \int \frac{dx}{2\pi} e^{iN/2-N} \langle \Psi(0) | \left( \prod_{\Gamma} D_{\Gamma}^{-1} \right) \left( \prod_{\rho} \left( 1 + e^{-iH(\Phi_{\rho})} p_\rho (x - p_\rho / 2) d_{r-p_\rho} D_{r_\rho} \right) D_{r_\rho^{-1}} D_{r_\rho^{-1}} \right) \left( \prod_{\Gamma'} \left( d_{r'-p'_\rho} D_{r'_\rho} d_{r'_\rho^{-1}} \right) \right) \left( \prod_{\Gamma'} D_{\Gamma'}^{-1} \right) | \Psi(0) \rangle \]

\[ \times \left( \prod_{r',s'} \left( d_{r'-p'_\rho} d_{r'_\rho} d_{r'_\rho^{-1}} \right) \right) \left( \prod_{r',s'} e^{iH(\Phi_{\rho})} p_{s' - p'_\rho / 2} (x - s' / 2) D_{r'_s} d_{r'_s^{-1}} \right) \left( \prod_{r'} D_{r'}^{-1} \right) | \Psi(0) \rangle \]

\[ + \langle \Psi(0) | \left( \prod_{r',s'} \left( d_{r'-p'_\rho} d_{r'_\rho} d_{r'_\rho^{-1}} \right) \right) \left( \prod_{r',s'} e^{iH(\Phi_{\rho})} p_{s' - p'_\rho / 2} (x - s' / 2) D_{r'_s} d_{r'_s^{-1}} \right) \left( \prod_{r'} D_{r'}^{-1} \right) | \Psi(0) \rangle \]

\[ = \int \frac{dx}{2\pi} e^{iN/2-N} \left( \prod_{\Gamma} D_{\Gamma}^{-1} \right) \left( \prod_{\rho} \left( 1 + e^{-iH(\Phi_{\rho})} p_\rho (x - p_\rho / 2) d_{r-p_\rho} D_{r_\rho} \right) D_{r_\rho^{-1}} D_{r_\rho^{-1}} \right) \left( \prod_{\Gamma'} \left( d_{r'-p'_\rho} D_{r'_\rho} d_{r'_\rho^{-1}} \right) \right) \left( \prod_{\Gamma'} D_{\Gamma'}^{-1} \right) | \Psi(0) \rangle \]

\[ \times \left( \prod_{r',s'} \left( d_{r'-p'_\rho} d_{r'_\rho} d_{r'_\rho^{-1}} \right) \right) \left( \prod_{r',s'} e^{iH(\Phi_{\rho})} p_{s' - p'_\rho / 2} (x - s' / 2) D_{r'_s} d_{r'_s^{-1}} \right) \left( \prod_{r'} D_{r'}^{-1} \right) | \Psi(0) \rangle \]

\[ + \langle \Psi(0) | \left( \prod_{r',s'} \left( d_{r'-p'_\rho} d_{r'_\rho} d_{r'_\rho^{-1}} \right) \right) \left( \prod_{r',s'} e^{iH(\Phi_{\rho})} p_{s' - p'_\rho / 2} (x - s' / 2) D_{r'_s} d_{r'_s^{-1}} \right) \left( \prod_{r'} D_{r'}^{-1} \right) | \Psi(0) \rangle \]

Almost identical reasoning yields the two-body matrix element,

\[ \langle \Psi_N | \hat{D}_{r,s} | \Psi_N \rangle = \int \frac{dx}{2\pi} e^{iN/2-N} \langle \Psi(0) | \left( \prod_{\Gamma} D_{\Gamma}^{-1} \right) \left( \prod_{\rho} \left( 1 + e^{-iH(\Phi_{\rho})} p_\rho (x - p_\rho / 2) d_{r-p_\rho} D_{r_\rho} \right) D_{r_\rho^{-1}} D_{r_\rho^{-1}} \right) \left( \prod_{\Gamma'} \left( d_{r'-p'_\rho} D_{r'_\rho} d_{r'_\rho^{-1}} \right) \right) \left( \prod_{\Gamma'} D_{\Gamma'}^{-1} \right) | \Psi(0) \rangle \]

\[ \times \left( \prod_{r',s'} \left( d_{r'-p'_\rho} d_{r'_\rho} d_{r'_\rho^{-1}} \right) \right) \left( \prod_{r',s'} e^{iH(\Phi_{\rho})} p_{s' - p'_\rho / 2} (x - s' / 2) D_{r'_s} d_{r'_s^{-1}} \right) \left( \prod_{r'} D_{r'}^{-1} \right) | \Psi(0) \rangle \]

\[ + \langle \Psi(0) | \left( \prod_{r',s'} \left( d_{r'-p'_\rho} d_{r'_\rho} d_{r'_\rho^{-1}} \right) \right) \left( \prod_{r',s'} e^{iH(\Phi_{\rho})} p_{s' - p'_\rho / 2} (x - s' / 2) D_{r'_s} d_{r'_s^{-1}} \right) \left( \prod_{r'} D_{r'}^{-1} \right) | \Psi(0) \rangle \]
The final needed matrix element is more subtle,

\[ \langle v_N(\mathbf{p}) | d_{r_1 s_1} | v_N(\mathbf{p'}) \rangle \]

\[ = \int \frac{d\mathbf{x}}{2\pi} e^{iN/2-N} \chi(\mathbf{x}) \det[G_{x,y}(\mathbf{r} - \mathbf{r'}, \mathbf{r} - \mathbf{r'}, t = 0^-) \epsilon_{ij}^{x+y}(x + i\Phi f^y h^x)(x')^{x'} + \epsilon_{ij}^{x+y}(x + i\Phi f^y h^x)(x')^{x'}, t = 0^+) (1 - \delta_{(r', s')_i(r_1 s_1)} - \delta_{(r', s')_i(r_2 s_2)})]. \]

The operators \( d_{r_1 s_1} \) and \( d_{r_2 s_2} \) get multiplied in the product rather than appearing in different terms, while \( d_{r_1 s_1} \) and \( d_{r_2 s_2} \) are both absent. All the destruction operators \( d_{r_1 s_1} \) on the other hand, arise in the usual fashion. We therefore see that

\[ \int \frac{d\mathbf{x}}{2\pi} e^{iN/2-N} \chi(\mathbf{x}) \det[G_{x,y}(\mathbf{r} - \mathbf{r'}, \mathbf{r} - \mathbf{r'}, t = 0^-) \epsilon_{ij}^{x+y}(x + i\Phi f^y h^x)(x')^{x'} + \epsilon_{ij}^{x+y}(x + i\Phi f^y h^x)(x')^{x'}, t = 0^+) (1 - \delta_{(r', s')_i(r_1 s_1)} - \delta_{(r', s')_i(r_2 s_2)})]. \]

where \( P \) is a permutation of the \( N_o \) locations \((r_i, s_i)\). Finally,

\[ = \int \frac{d\mathbf{x}}{2\pi} e^{iN/2-N} \chi(\mathbf{x}) \det[G_{x,y}(\mathbf{r} - \mathbf{r'}, \mathbf{r} - \mathbf{r'}, t = 0^-) \epsilon_{ij}^{x+y}(x + i\Phi f^y h^x)(x')^{x'} + \epsilon_{ij}^{x+y}(x + i\Phi f^y h^x)(x')^{x'}, t = 0^+) (1 - \delta_{(r', s')_i(r_1 s_1)} - \delta_{(r', s')_i(r_2 s_2)})]. \]
The matrix element formulas (13) arise upon definition of the matrices should they be required for a microscopic Hamiltonian other than (1).

\[ -G_{x,x'}(\mathbf{r} - \mathbf{p}', \mathbf{r}' - \mathbf{p}', t = 0^+) \delta_{(x',x')}(\mathbf{r}, \mathbf{r}') + \left[ G_{x,x'}(\mathbf{r} - \mathbf{p}', \mathbf{r}' - \mathbf{p}, t = 0^+) e^{i\mathbf{s}(\mathbf{p}/|\mathbf{p}|)} (|\mathbf{p}'(\mathbf{r}' - \mathbf{p}';2) - \mathbf{p}(\mathbf{r} - \mathbf{p}/2)|) \right] \]

\[ -G_{x,x'}(\mathbf{r} - \mathbf{p}', \mathbf{r}' - \mathbf{p}', t = 0^+) \left[ 1 - \delta_{(x',x')}(\mathbf{r}, \mathbf{r}') - \delta_{(x',x')}(\mathbf{r}, \mathbf{r}') \right]. \]

The matrix element formulas (13) arise upon definition of the matrices should they be required for a microscopic Hamiltonian other than (1).