Berry Phase Effect on Semiclassical Dynamics of Bogoliubov Quasiparticles

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We develop a semiclassical theory for Bogoliubov quasiparticles in a superfluid by following the center of mass motion of a quasiparticle wavepacket. Berry phase arises when the underlying condensate moves, invalidating the usual canonical relation between the mechanical momentum and position variables. The equations of motion become non-Hamiltonian, and the quantization rule and the density of states are also modified. As an application of our semiclassical theory, we study quasiparticles in a condensate with a vortex to show explicitly the Berry phase effects.

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Newtonian dynamics and geometric optics have provided a simple and effective world view of matter and light, and the classical concepts such as trajectories or rays have continued to play a prominent role in early formulation of wave optics and quantum mechanics. In retrospect, after the full development of wave mechanics, the classical concepts are seen to be naturally born out in approximate solutions to the wave equations in appropriate limits. Today, because of its transparent view on physical quantities and processes, the semiclassical approach to wave equations has become an essential tool in all branches of physics [1, 2].

In recent years, there has been intense interest in the dynamics of Bose-Einstein condensates (BEC) of ultracold atoms [3]. The elementary excitations are described by linear wave equations known as Bogoliubov equations, which differ essentially from the Schrödinger equation because of interactions between the atoms. Besides numerical and perturbative approaches [3, 4, 5, 6, 7], one naturally appeals to the semiclassical method which maps the Bogoliubov equations to more intuitive Hamiltonian equations of motion for the position and mechanical momentum of quasiparticles [8, 9, 10, 11]. For condensates in various traps where these classical equations are integrable, quasiparticle energy levels have been obtained by Bohr-Sommerfeld quantization rule, and their wavefunctions by the standard Wentzel-Kramers-Brillouin (WKB) approximation. However, the validity of this approach is limited to the case with ground state condensates, and essential modifications must be introduced for condensates with a flow such as in the presence of vortices or for condensates in periodic potentials.

In this Letter, we develop a semiclassical theory for Bogoliubov waves by following the center of mass motion of a wavepacket in the phase space of position and mechanical momentum. We find that Berry phase [12] arises whenever the underlying condensate flows, which renders the quasiparticle mechanical momentum non-canonical in relation to the position variable. As a result, the equations of motion for the mechanical momentum and position become non-Hamiltonian, and an extra Berry phase term appears in the semiclassical quantization rule. In addition, the Berry phase modifies the Liouville's theorem on the conservation of phase space volume, and introduces a correction to the density of states of quasiparticles [13]. To demonstrate the utility of our theory, we study quasiparticles in a condensate with a vortex, where these Berry phase effects are shown explicitly.

Wavepacket dynamics— Although our theory can be easily generalized to the situation with a fast-varying periodic potential [14], we choose to present it here for the simpler case with a slowly varying trapping potential for which general analytical formulas are found. The dynamics of a superfluid condensate is described by the Gross-Pitaveskii equation [15]

$$i\hbar\frac{\partial\psi_0}{\partial t}=\left(\frac{\mathbf{p}^2}{2m}+g\left|\psi_0\right|^2+V\left(\mathbf{r}\right)-\mathbf{\Omega}\cdot\left(\mathbf{r}\times\mathbf{p}\right)\right)\psi_0, \quad (1)$$

where $g=4\pi\hbar^2 a_s/m$ is the inter-atom coupling constant with the s-wave scattering length a_s, and $V\left(\mathbf{r}\right)$ is the trapping potential. We have also included an angular momentum term to take into account the possibility of using a rotating reference frame, with $\mathbf{\Omega}$ being its angular frequency. The condensate wavefunction may be written as $\psi_0=\sqrt{n\left(\mathbf{r}\right)}e^{i\alpha(\mathbf{r})}e^{-i\mu t}$, where μ is the chemical potential, $n\left(\mathbf{r}\right)$ and $\alpha\left(\mathbf{r}\right)$ are the condensate density and phase respectively. A nonzero gradient of phase corresponds to a flow of the condensate $\mathbf{v}_s=\nabla\alpha\left(\mathbf{r}\right)$.

Small deviation $\delta\psi e^{-i\mu t}$ (elementary excitations) from the condensate wavefunction ψ_0 is described by the Bogoliubov equation [15]

$$i\sigma_z\frac{\partial}{\partial t}\left|\Phi\right\rangle=\mathcal{Q}\left|\Phi\right\rangle,\ \mathcal{Q}=\begin{pmatrix}H_+ & H_2e^{2i\alpha(\mathbf{r})}\\ H_2e^{-2i\alpha(\mathbf{r})} & H_-\end{pmatrix}, \quad (2)$$

where for simpler notation we have used units such that $\hbar$ and the atomic mass m are both unity. The wavefunction Φ has two components, u and v, which are related to $\delta\psi$ through $\delta\psi=ue^{-i\omega t}+v^*e^{i\omega t}$, where ω is the quasiparticle energy. The entries of the matrix operator are given by $H_\pm=\mathbf{p}^2/2+2gn\left(\mathbf{r}\right)+V\left(\mathbf{r}\right)-\mu\mp\mathbf{\Omega}\cdot\left(\mathbf{r}\times\mathbf{p}\right)$, and $H_2\left(\mathbf{r}\right)=gn\left(\mathbf{r}\right)$. Because of the Pauli matrix σ_z on the left hand side, the Bogoliubov equation is nonhermitian.

We now consider a quasiparticle wavepacket centered at $\mathbf{r}_c$ with its spread small compared to the length scale of the slowly varying potentials (including trap potential $V(\mathbf{r})$, condensate wavefunction ψ_0 and terms related to $\boldsymbol{\Omega}$). The dynamics of the wavepacket is approximately governed by the local Bogoliubov operator $\mathcal{Q}_c \equiv \mathcal{Q}(\mathbf{p}, \mathbf{r} = \mathbf{r}_c)$ plus its gradient correction $\mathcal{Q} \approx \mathcal{Q}_c + \frac{1}{2}\left((\mathbf{r}-\mathbf{r}_c)\cdot\frac{\partial \mathcal{Q}_c}{\partial \mathbf{r}_c} + c.c\right)$. The gradient term is small in the neighborhood of the wavepacket and may be treated perturbatively. The local Bogoliubov operator has plane wave eigenstates

$$\mathcal{Q}_c e^{i\mathbf{q}\cdot\mathbf{r}} \left|\phi(\mathbf{q},\mathbf{r}_c)\right\rangle = \omega_c \sigma_z e^{i\mathbf{q}\cdot\mathbf{r}} \left|\phi(\mathbf{q},\mathbf{r}_c)\right\rangle, \tag{3}$$

where $\mathbf{q}$ is the wavevector. The amplitude satisfies a simple 2x2 matrix equation, which can be solved easily to yield

$$\omega_c = \left(H_1^2 - H_2^2\right)^{1/2} + \mathbf{q}\cdot(\boldsymbol{\Omega}\times\mathbf{r}_c) \tag{4}$$

for the local quasiparticle energy, where $H_1 = \frac{\mathbf{q}^2}{2m} + 2gn(\mathbf{r}_c) + V(\mathbf{r}_c) - \mu$, and

$$\left|\phi(\mathbf{q},\mathbf{r}_c)\right\rangle = \frac{1}{2}\begin{pmatrix} \zeta+\zeta^{-1} \\ \left(\zeta-\zeta^{-1}\right)e^{-2i\alpha(\mathbf{r}_c)} \end{pmatrix} \tag{5}$$

for the two-component amplitude of the local eigenstate, where $\zeta = \left(\frac{H_1-H_2}{H_1+H_2}\right)^{1/4}$. We note that the wavevector $\mathbf{q}$ and the wavepacket center $\mathbf{r}_c$ enter the local quasiparticle energy and wavefunction parametrically. The wavefunction is normalized in a sense that $\left\langle\phi(\mathbf{q},\mathbf{r}_c)\right|\sigma_z\left|\phi(\mathbf{q},\mathbf{r}_c)\right\rangle = 1$. We have also chosen the phase of the wavefunction such that it is smooth and single valued in the parameters $(\mathbf{q},\mathbf{r}_c)$. We shall see that the parametric dependence of the eigenstates on the center position of the wavepacket will manifest as Berry-phase terms in the semiclassical equations of motion.

We now turn our attention to the wavepacket itself, which is to be constructed out of these eigenstates as

$$|\Phi\rangle = \int d^3q\, a(\mathbf{q},t)\, e^{i\mathbf{q}\cdot\mathbf{r}} \left|\phi(\mathbf{q},\mathbf{r}_c)\right\rangle, \tag{6}$$

where the superposition amplitude $a(\mathbf{q},t)$ may be taken as a Gaussian in $\mathbf{q}$. The normalization is taken to be $\langle\Phi|\sigma_z|\Phi\rangle = \int d^3q \left|a(\mathbf{q},t)\right|^2 = 1$. We assume that the Gaussian is centered at $\mathbf{q}_c$ and has a width narrow compared to momentum scales of the energy dispersion and of the eigenstates. Microscopic calculation shows that $\mathbf{q}_c = \langle\Phi|\sigma_z\mathbf{p}|\Phi\rangle = \int \delta\psi^*\mathbf{p}\delta\psi d\mathbf{r}$ is the mechanical momentum of the quasiparticle [14]. To be self consistent, the wavepacket must yield the preassigned center position $\mathbf{r}_c = \langle\Phi|\sigma_z\mathbf{r}|\Phi\rangle$. Finally, the dynamics of the wavepacket can be derived from a time-dependent variational principle for the Bogoliubov equation, with the Lagrangian given by

$$L = \langle\Phi|\, i\sigma_z \frac{d}{dt}\, |\Phi\rangle - \langle\Phi|\,\mathcal{Q}\,|\Phi\rangle. \tag{7}$$

We use d/dt to mean the derivative with respect to the time dependence of the wavefunction explicitly or implicitly through the parameters $\mathbf{r}_c$ and $\mathbf{q}_c$. Under the previously discussed conditions that the wavepacket is narrow both in position and momentum spaces, the Lagrangian can be evaluated as a function of $\mathbf{r}_c$ and $\mathbf{q}_c$, and their time derivatives, independent of the width and shape of the wavepacket in position or momentum.

We now summarize our results, leaving the details of derivation to a future publication [14]. We find that the Lagrangian takes the form

$$L = -\omega_c - \Delta\omega + (\mathbf{q}_c + \mathbf{A})\cdot\dot{\mathbf{r}}_c. \tag{8}$$

Apart from the local eigenenergy ω_c, the wavepacket energy has a correction $\Delta\omega = \left(1-\rho^2\right)\mathbf{q}_c\cdot\nabla\alpha(\mathbf{r}_c)$ from the gradient expansion of the Bogoliubov operator, where $\rho = \langle\phi|\phi\rangle$ is equal to the atom density in the eigenstate. There is also a vector potential $\mathbf{A} = i\langle\phi|\sigma_z|\partial\phi/\partial\mathbf{r}_c\rangle = -(\rho-1)\nabla\alpha(\mathbf{r}_c)$, whose line integral over a path gives a Berry phase of the eigenstate. The effect of Berry phase has been extensively studied for semiclassical electron transport in crystals [16], and the theory has been extended to amend geometric optics in smoothly inhomogeneous media [17] and in photonic crystals [18].

The Euler-Lagrangian equations then yield the equations of motion for the center position and mechanical momentum,

$$\begin{aligned}
\dot{\mathbf{r}}_c &= \frac{\partial\omega}{\partial\mathbf{q}_c} - \frac{\partial\left(\mathbf{A}\cdot\dot{\mathbf{r}}_c\right)}{\partial\mathbf{q}_c}, \\
\dot{\mathbf{q}}_c &= -\frac{\partial\omega}{\partial\mathbf{r}_c} + \dot{\mathbf{r}}_c\times(\nabla\times\mathbf{A}) - \left(\dot{\mathbf{q}}_c\cdot\frac{\partial}{\partial\mathbf{q}_c}\right)\mathbf{A}.
\end{aligned} \tag{9}$$

Here $\omega = \omega_c + \Delta\omega$ is the quasiparticle energy, and the $\mathbf{q}_c$ derivative is done with $\dot{\mathbf{r}}_c$ fixed. These equations are not of Hamiltonian form, and they differ from the classical Hamilton's equations obtained from the WKB method [8, 9, 10, 11] in two aspects. Firstly, the energy ω contains a correction term $\Delta\omega$ in the presence of a flow of the condensate. Secondly, the phase associated with the flow of the condensate induces a vector potential $\mathbf{A}$ for quasiparticles, which yields Berry phase corrections to the equations of motion (9).

Quantum properties of the Bogoliubov equation, such as discrete energy levels, can be obtained through quantization of the classical orbits. For a regular orbit, the discrete energy levels can be obtained using the Einstein-Brillouin-Keller quantization procedure $\oint_{\mathcal{C}}\mathbf{k}_c\cdot d\mathbf{r}_c = 2\pi\left(l+\frac{\nu}{4}\right)$, where $\mathcal{C}$ denotes an orbit of constant energy ω, l is an integer that labels the eigenvalue, ν is the number of caustics traversed, and $\mathbf{k}_c = \mathbf{q}_c + \mathbf{A}$ is the canonical momentum conjugate to the coordinate vector $\mathbf{r}_c$. The above quantization rule yields

$$\oint_{\mathcal{C}}\mathbf{q}_c\cdot d\mathbf{r}_c = 2\pi\left(l+\frac{\nu}{4}\right) - \Gamma(\mathcal{C}), \tag{10}$$

where $\Gamma(\mathcal{C}) = \oint_{\mathcal{C}} d\mathbf{r}_c \cdot \mathbf{A} = -\oint_{\mathcal{C}} (\rho - 1)\, d\alpha(\mathbf{r}_c)$ is the Berry phase acquired by the wavepacket upon going round the closed orbit once. Consider a quasiparticle moving adiabatically around a vortex, Bijlsma and Stoof showed several years ago that the accumulated Berry phase is $-\oint_{\mathcal{C}} \rho d\alpha(\mathbf{r}_c)$ [19], which has 2π difference from our result.

In classical Hamiltonian dynamics, Liouville's theorem states that the phase space volume is conserved, and conventionally the density of state is taken as the constant $1/(2\pi)^3$. The Berry phase makes the equations of motion non-Hamiltonian, rendering the violation of Liouville's theorem and modifying the density of states of quasiparticles to [13]

$$D = \det\left(I - \frac{\partial \mathbf{A}}{\partial \mathbf{q}_c}\right) / (2\pi)^3, \tag{11}$$

where I is the 3×3 unit matrix, and $\left(\frac{\partial \mathbf{A}}{\partial \mathbf{q}_c}\right)_{\alpha\beta} = -\frac{\partial \rho}{\partial q_\alpha} \frac{\partial \alpha(\mathbf{r}_c)}{\partial r_{c\beta}}$ is a Berry curvature.

We emphasize here that these effects of Berry phase are important only in low and intermediate energy regions and vanish in high energy region ($\rho \to 1$), where quasiparticles become free particles and their properties are independent of the condensate.

Canonical formulation — We see that the semiclassical quantization rule becomes simpler by introducing the canonical momentum $\mathbf{k}_c = \mathbf{q}_c - (\rho - 1)\nabla\alpha(\mathbf{r}_c)$ in place of the mechanical momentum $\mathbf{q}_c$. Similarly, the equations of motion (9) can also be simplified to the Hamiltonian form,

$$\dot{\mathbf{r}}_c = \frac{\partial \omega}{\partial \mathbf{k}_c}, \dot{\mathbf{k}}_c = -\frac{\partial \omega}{\partial \mathbf{r}_c}. \tag{12}$$

The quasiparticle energy is now a function of the canonical momentum, given by

$$\omega = \left[H_1^2 - H_2^2\right]^{\frac{1}{2}} + (\mathbf{k}_c - \mathbf{A}) \cdot (\mathbf{\Omega} \times \mathbf{r}_c) + \mathbf{k}_c \cdot \mathbf{A}. \tag{13}$$

At this stage it will be instructive to consider the situation of a uniformly flowing superfluid of velocity $\mathbf{v}_s$, and compare our quasiparticle energy dispersion with that obtained using Galilean invariance. If $\mathbf{p}_0$ is the quasiparticle momentum in the reference frame where the superfluid is static, then its energy in the laboratory reference frame is found by Galilean transformation to be [20]

$$\omega = \varepsilon(\mathbf{p}_0) + \mathbf{p}_0 \cdot \mathbf{v}_s, \tag{14}$$

where $\varepsilon(\mathbf{p}_0) = \left[\frac{p_0^2}{2}\left(\frac{p_0^2}{2} + 2gn\right)\right]^{1/2}$ is the energy dispersion in a static superfluid. This result can also be obtained from our energy dispersion Eq. (13) by setting $\mathbf{p}_0 = \mathbf{k}_c - \mathbf{v}_s = \mathbf{q}_c - \rho\mathbf{v}_s$ and expanding to first order in $\mathbf{v}_s$. The last equality shows that the quasiparticle mechanical momentum $\mathbf{q}_c$ in a moving superfluid differs from its momentum $\mathbf{p}_0$ in the co-moving frame of the superfluid by the amount $\rho\mathbf{v}_s$, which is quite a reasonable result because ρ is the total atomic mass contained in the quasiparticle wavepacket.

Although the physical significance of our canonical momentum $\mathbf{k}_c$ is not clear, we can use it to simplify calculations in many problems. Here we apply the semiclassical quantization rule to calculate the quasiparticle energy levels in the presence of a trapped vortex [21, 22]. For simplicity, we consider a quasi-two-dimensional symmetric trap with strong confinement along the $\hat{\mathbf{z}}$ direction. Here we only sketch the steps for the calculation, leaving the numerical results to a future publication [14].

Because of the rotational symmetry of the system, the wavefunction of the vortex can be written as $\psi(\mathbf{r}) = \sqrt{n(r)}e^{i\theta}$, where θ is the azimuthal angle, r is the radius on the xy plane. In addition to the previous choice of $\hbar = m = 1$, we choose the energy unit such that the chemical potential $\mu = 1$. The rotational symmetry yields conserved canonical angular momentum $J_z = (\mathbf{r}_c \times \mathbf{k}_c)_z$. The canonical momentum for the radial coordinate r_c can be written as $P_r(r_c, J_z, E) = \left(k_c^2(r_c) - J_z^2/r_c^2\right)^{1/2}$, where $k_c(r_c)$ can be determined from the conservation of energy $E = \omega_c + \Omega(J_z + \rho - 1) + J_z(1-\rho)/r_c^2$ with the local quasiparticle energy $\omega_c = \left[\left(k_c^2/2 + 2n - 1 + V\right)^2 - n^2\right]^{1/2}$ and the atom density $\rho = \left(1 + n^2/\omega_c^2\right)^{1/2}$. To determine the energy levels of quasiparticles, we use quantized angular momentum $J_z = j$, and the quantization rule Eq. (10) reduces to

$$\int_{r_<}^{r_>} P_r(r_c, J_z, E)\, dr_c = \pi\left(l + \frac{1}{2}\right), \tag{15}$$

where $r_<$ and $r_>$ are classical turning points at which the integrand becomes zero, and j, l are integers. Numerically solving the implicit expression (15) for E for different values of the integers l and j, we can obtain the quasiparticle energy levels [14].

We emphasize that it is important to distinguish physical and canonical quantities in the investigation of quasiparticle dynamics, because the Berry phase makes them different in many problems. For instance, the mechanical angular momentum of the quasiparticles in the above problem, given by $(\mathbf{r}_c \times \mathbf{q}_c)_z = J_z + (\rho - 1)$, is different from the canonical angular momentum J_z. In noncircular orbits, the mechanical angular momentum is not conserved.

Momentum circulation — To further illustrate the difference between canonical and mechanical momenta, we calculate the momentum circulation of quasiparticles in equilibrium around a vortex in an infinite uniform superfluid. This quantity characterizes the quasiparticle contribution to the transverse Magnus force acting on a moving vortex [23].

The momentum density of quasiparticles under equilibrium Bose-Einstein distribution is obtained by summing over the mechanical momenta from all states (labelled by the canonical momentum),

$$\mathbf{W} = \int \frac{d^3\mathbf{k}_c}{(2\pi)^3} \frac{\mathbf{k}_c + (\rho - 1)\nabla\theta_c}{e^{\omega(\mathbf{r}_c,\mathbf{k}_c)/k_BT} - 1} \tag{16}$$
$$= \int d^3\mathbf{q}_c \frac{D(\mathbf{r}_c, \mathbf{q}_c)}{(2\pi)^3} \frac{\mathbf{q}_c}{e^{\omega(\mathbf{r}_c,\mathbf{q}_c)/k_BT} - 1},$$

where T is the temperature, k_B is the Boltzman constant, $1/(2\pi)^3$ is the density of states for the canonical momentum $\mathbf{k}_c$, and

$$D(\mathbf{r}_c, \mathbf{q}_c) = 1 + \frac{1-\rho^2}{\omega_c r_c^2}(\mathbf{r}_c \times \mathbf{q}_c)_z \tag{17}$$

is the Jacobian for the variable transformation. We notice that $D(\mathbf{r}_c, \mathbf{q}_c)/(2\pi)^3$ is actually the modified density of states obtained from Eq. (11) for the non-canonical momentum $\mathbf{q}_c$. This formula shows that the density of states for quasiparticles moving along the vortex flow is smaller than that opposing the flow.

The transverse force contributed by quasiparticles on a moving vortex with velocity $\mathbf{v}$ is [23]

$$\mathbf{F} = \kappa(\mathcal{C})\, \mathbf{v} \times \hat{\mathbf{z}}, \tag{18}$$

where $\kappa(\mathcal{C}) = \oint_{\mathcal{C}} \mathbf{W} \cdot d\mathbf{r}_c$ is the momentum circulation at large radius around a stationary vortex. Since we choose the orbit $\mathcal{C}$ to be well away from the core of the vortex, we can expand $f(\mathbf{k}_c) \approx f_0(\mathbf{k}_c) - \Delta f$ with $f_0(\mathbf{k}_c) = \frac{1}{e^{\omega_c/k_BT}-1}$, and $\Delta f = \frac{e^{\omega_c/k_BT}}{\left(e^{\omega_c/k_BT}-1\right)^2} \frac{(1-\rho)\mathbf{k}_c \cdot \nabla\theta_c}{k_BT}$. Considering a closed orbit with fixed radius R and taking the limit $R \to \infty$, we find that there are two nonzero terms in the circulation

$$\kappa(\mathcal{C}) = \int_0^\infty f_0(\mathbf{k}_c)\, \rho k_c^2 dk_c \tag{19}$$
$$- \frac{1}{3k_BT} \int_0^\infty \frac{e^{\omega_c/k_BT} k_c^4 dk_c}{\left(e^{\omega_c/k_BT} - 1\right)^2}.$$

The first term stems from the difference between the canonical momentum $\mathbf{k}_c$ and mechanical momentum $\mathbf{q}_c$, while the second term comes from the deviation Δf in the distribution function. The first term represents the total atomic number density ρ contained in the quasiparticles and has a T^2 temperature dependence. Interestingly, this term compensates the decrease in the superfluid circulation caused by the depletion of the condensate at finite temperatures [20]. The remaining quasiparticle circulation goes as T^4. However, it is not clear whether this T^4 dependence can also be canceled by higher order terms in the superfluid circulation.

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